International School on Fundamental Crystallography

and

Workshop on Structural Phase Transitions

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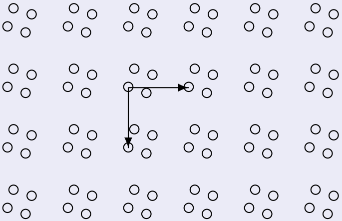
Crystallographic space groups.

Overview

- lattices and their properties
- point groups of space groups
- coset decomposition with respect to the translation subgroup
- interplay between lattices and point groups
- glide reflections and screw rotations
- symmorphic and non-symmorphic space groups

Periodic patterns



- A 3D (2D) periodic crystal pattern is invariant under translations in three (two) independent directions.
- The translations leaving a periodic crystal pattern invariant are closed under taking integral linear combinations.

Definition

For vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ forming a basis of $\mathbb{R}^3$, the set of all integral linear combinations

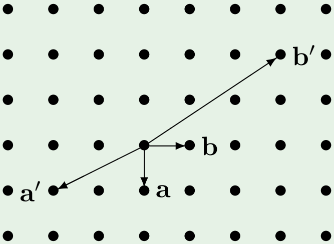
$$\mathbf{L} = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$$

is called a lattice in $\mathbb{R}^3$ and $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a lattice basis of $\mathbf{L}$.

Basic properties of lattices

- The translation vectors of a periodic crystal pattern form a lattice.
- For a vector $\mathbf{v} = x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$, the column $\begin{pmatrix} x \\ y \\ z \end{pmatrix}$ is called the coordinate column of $\mathbf{v}$ with respect to $\mathbf{a}, \mathbf{b}, \mathbf{c}$
- A lattice has infinitely many bases: for an integral 3×3-matrix $\mathbf{P}$ with $\det \mathbf{P} = \pm 1$, also the inverse matrix $\mathbf{P}^{-1}$ is an integral matrix.
- In this case, also $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\mathbf{P}$ is a lattice basis of $\mathbf{L}$, since the original basis vectors can be expressed as integral linear combinations of the new basis: $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\mathbf{a}', \mathbf{b}', \mathbf{c}')\mathbf{P}^{-1}$.

Example



$$\mathbf{a}' = \mathbf{a} - 2\mathbf{b}$$

$$\mathbf{b}' = -2\mathbf{a} + 3\mathbf{b}$$

$$\mathbf{c}' = \mathbf{c}$$

$$\mathbf{P} = \begin{pmatrix} 1 & -2 & 0 \\ -2 & 3 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathbf{P}^{-1} = \begin{pmatrix} -3 & -2 & 0 \\ -2 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow \mathbf{a} = -3\mathbf{a}' - 2\mathbf{b}', \ \mathbf{b} = -2\mathbf{a}' - \mathbf{b}', \ \mathbf{c} = \mathbf{c}'$$

Metric properties

- $\mathbb{R}^3$ is turned into a Euclidean space $\mathbb{E}^3$ by the (Pythagorean) length $|\mathbf{v}| = \sqrt{v_x^2 + v_y^2 + v_z^2}$ and the corresponding scalar product $\mathbf{v} \cdot \mathbf{w} = v_x w_x + v_y w_y + v_z w_z$
- Angles can be computed by $\cos \measuredangle(\mathbf{v}, \mathbf{w}) = \dfrac{\mathbf{v} \cdot \mathbf{w}}{|\mathbf{v}|\ |\mathbf{w}|}$.

Metric tensor

- The matrix $\boldsymbol{G} = \begin{pmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix}$ containing the scalar products of the lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is called the metric tensor of $\mathbf{L}$.
- Computing scalar products from coordinate columns:

$$\mathbf{v} = x_1\mathbf{a} + y_1\mathbf{b} + z_1\mathbf{c}, \qquad \mathbf{w} = x_2\mathbf{a} + y_2\mathbf{b} + z_2\mathbf{c}$$

$$\Rightarrow \mathbf{v} \cdot \mathbf{w} = (x_1\ y_1\ z_1) \cdot \boldsymbol{G} \cdot \begin{pmatrix} x_2 \\ y_2 \\ z_2 \end{pmatrix}$$

Quick quiz

Determine the metric tensor of the lattice $\mathbf{L}$ with lattice basis

$$\mathbf{a} = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

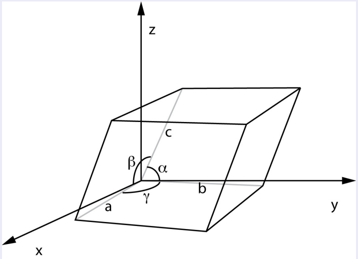
Can you say something about the type of this lattice?

Answer

$$\boldsymbol{G} = \begin{pmatrix} 6 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

This is an orthorhombic lattice.

Unit cell



- The parellelepiped $\{x\mathbf{a} + y\mathbf{b} + z\mathbf{c} \mid 0 \leq x, y, z < 1\}$ spanned by the lattice basis of $\mathbf{L}$ is called the primitive unit cell of $\mathbf{L}$.
- The lengths a, b, c of the basis vectors and the angles α, β, γ between them are called the cell parameters.
- Metric tensor $\boldsymbol{G} = \begin{pmatrix} a^2 & ab\cos\gamma & ac\cos\beta \\ ab\cos\gamma & b^2 & bc\cos\alpha \\ ac\cos\beta & bc\cos\alpha & c^2 \end{pmatrix}$, i.e. the cell parameters can be read off the metric tensor and vice versa.
- The volume of the unit cell is

$$V = \sqrt{\det \boldsymbol{G}} = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c}) = \mathbf{b} \cdot (\mathbf{c} \times \mathbf{a}) = \mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})$$

Primitive and centered lattices

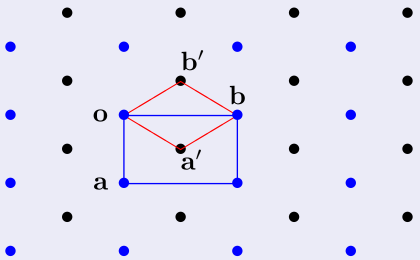
Conventional basis

- Basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ with particularly nice metric properties (e.g. vectors perpendicular to each other).
- Basis vectors are along symmetry directions of the lattice.
- $\mathbf{L}_p = \{l\mathbf{a} + m\mathbf{b} + n\mathbf{c} \mid l, m, n \in \mathbb{Z}\}$ lattice of integral linear combinations of the conventional basis, two cases:

  (1) primitive lattice: $\mathbf{L} = \mathbf{L}_p$

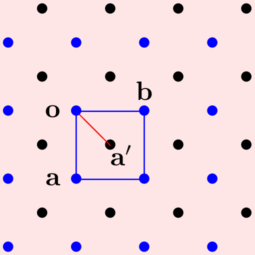
  (2) centred lattice: $\mathbf{L} = \mathbf{L}_P \cup (\mathbf{v}_2 + \mathbf{L}_P) \cup \ldots \cup (\mathbf{v}_s + \mathbf{L}_P)$ for centring vectors $\mathbf{v}_2, \ldots, \mathbf{v}_s$ (take $\mathbf{v}_1 = \mathbf{o}$)
- coset decomposition: $\mathbf{L}_p$ is a sublattice of index s in $\mathbf{L}$

Example: centred rectangular lattice



- conventional basis $\mathbf{a}, \mathbf{b}$
- centring vector $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$
- • nodes: primitive rectangular lattice $\mathbf{L}_p$ with primitive basis $\mathbf{a}, \mathbf{b}$
- • and • nodes: centred rectangular lattice $\mathbf{L} = \mathbf{L}_p \cup (\mathbf{a}' + \mathbf{L}_p)$ with primitive basis $\mathbf{a}', \mathbf{b}'$
- red cell: primitive cell for centred lattice $\mathbf{L}$
  blue cell: centred cell for centred lattice $\mathbf{L}$, primitive cell for primitive lattice $\mathbf{L}_p$

Exercise



Show that a centred square lattice with centring vector $\mathbf{a}' = \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}$ is again a square lattice.

What is the relation between the cell parameters of the primitive and the centred unit cell?

(For a 2D lattice, the cell parameters are the lengths a, b of the basis vectors $\mathbf{a}$, $\mathbf{b}$ and the angle γ between them.)

Answer

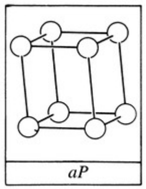
A primitive basis of the centred lattice is

$$\mathbf{a}' = \tfrac{1}{2}\mathbf{a} + \tfrac{1}{2}\mathbf{b},\ \mathbf{b}' = -\tfrac{1}{2}\mathbf{a} + \tfrac{1}{2}\mathbf{b}.$$

From $\mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} = a^2$ and $\mathbf{a}\cdot\mathbf{b} = 0$, we compute that $\mathbf{a}'\cdot\mathbf{a}' = \mathbf{b}'\cdot\mathbf{b}' = \frac{1}{2}a^2$ and $\mathbf{a}'\cdot\mathbf{b}' = 0$, hence the lattice is again a square lattice with $a' = \frac{1}{\sqrt{2}}a$.

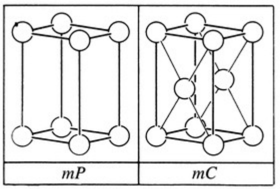
Description of lattice types and their centrings

Triclinic (anorthic)



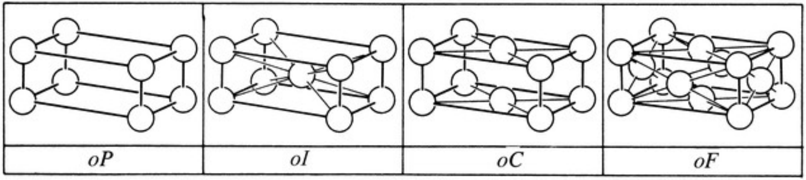
- metric tensor for conventional basis: $\boldsymbol{G} = \begin{pmatrix} g_{11} & g_{12} & g_{13} \\ & g_{22} & g_{23} \\ & & g_{33} \end{pmatrix}$
- 6 free parameters: a, b, c, α, β, γ
- no centrings

Monoclinic



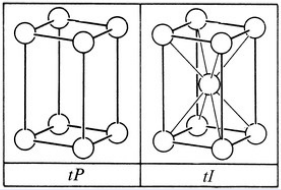
- metric tensor for conventional cell: $\boldsymbol{G} = \begin{pmatrix} g_{11} & 0 & g_{13} \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$
- 4 free parameters: a, b, c, β, $\alpha = \gamma = 90°$
- face-centred mC: centring vector $(\frac{1}{2}, \frac{1}{2}, 0)$

Orthorhombic



- metric tensor for conventional cell: $\boldsymbol{G} = \begin{pmatrix} g_{11} & 0 & 0 \\ & g_{22} & 0 \\ & & g_{33} \end{pmatrix}$
- 3 free parameters: a, b, c, $\alpha = \beta = \gamma = 90^\circ$
- body-centred oI: centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- face-centred oC: centring vector $(\frac{1}{2}, \frac{1}{2}, 0)$
- all-face-centred oF: centring vectors $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(0, \frac{1}{2}, \frac{1}{2})$

Tetragonal

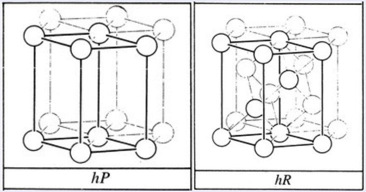


- metric tensor for conventional cell: $\boldsymbol{G} = \begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{33} \end{pmatrix}$
- 2 free parameters: $a = b$, c, $\alpha = \beta = \gamma = 90°$
- body-centred tI: centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Quick quiz

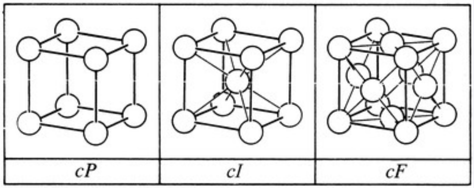
Why is there no face-centred tetragonal lattice?

Hexagonal



- metric tensor for conventional cell: $\boldsymbol{G} = \begin{pmatrix} 2g_{11} & -g_{11} & 0 \\ & 2g_{11} & 0 \\ & & g_{33} \end{pmatrix}$
- 2 free parameters: $a = b$, c, $\alpha = \beta = 90°$, $\gamma = 120°$
- rhombohedrally centred hR: centring vectors $(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$, $(\frac{1}{3}, \frac{2}{3}, \frac{2}{3})$

Cubic



- metric tensor for conventional cell: $\boldsymbol{G} = \begin{pmatrix} g_{11} & 0 & 0 \\ & g_{11} & 0 \\ & & g_{11} \end{pmatrix}$
- 1 free parameter: $a = b = c$, $\alpha = \beta = \gamma = 90°$
- body-centred cI: centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- face-centred cF: centring vectors $(\frac{1}{2}, \frac{1}{2}, 0)$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(0, \frac{1}{2}, \frac{1}{2})$

Reciprocal lattice

Motivation from diffraction analysis

- A diffraction pattern can be interpreted as the Fourier transform of the crystal pattern.
- Bragg-peaks are invariant under a translation by $\mathbf{w}^*$ if $e^{2\pi i \mathbf{v}\cdot\mathbf{w}^*} = 1$ for all $\mathbf{v} \in \mathbf{L} \Rightarrow \mathbf{v}\cdot\mathbf{w}^* \in \mathbb{Z}$ for all $\mathbf{v} \in \mathbf{L}$.

Definition

- For a lattice $\mathbf{L}$ in Euclidean space $\mathbb{E}^3$, the reciprocal lattice $\mathbf{L}^*$ of $\mathbf{L}$ is defined as $\mathbf{L}^* = \{\mathbf{w}^* \in \mathbb{E}^3 \mid \mathbf{v}\cdot\mathbf{w}^* \in \mathbb{Z} \text{ for all } \mathbf{v} \in \mathbf{L}\}$.
- If $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is a lattice basis of $\mathbf{L}$, a basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of $\mathbf{L}^*$ is determined by the properties:

$$\mathbf{a}\cdot\mathbf{a}^* = \mathbf{b}\cdot\mathbf{b}^* = \mathbf{c}\cdot\mathbf{c}^* = 1$$

$$\mathbf{a}\cdot\mathbf{b}^* = \mathbf{b}\cdot\mathbf{a}^* = \mathbf{b}\cdot\mathbf{c}^* = \mathbf{c}\cdot\mathbf{b}^* = \mathbf{c}\cdot\mathbf{a}^* = \mathbf{a}\cdot\mathbf{c}^* = 0$$

- This basis of $\mathbf{L}^*$ is called the reciprocal basis of $\mathbf{a}, \mathbf{b}, \mathbf{c}$.

Matrix characterization of the reciprocal basis

The reciprocal basis $\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*$ of $\mathbf{a}, \mathbf{b}, \mathbf{c}$ can conveniently be characterized by the matrix equation

$$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a}^* & \mathbf{a}\cdot\mathbf{b}^* & \mathbf{a}\cdot\mathbf{c}^* \\ \mathbf{b}\cdot\mathbf{a}^* & \mathbf{b}\cdot\mathbf{b}^* & \mathbf{b}\cdot\mathbf{c}^* \\ \mathbf{c}\cdot\mathbf{a}^* & \mathbf{c}\cdot\mathbf{b}^* & \mathbf{c}\cdot\mathbf{c}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

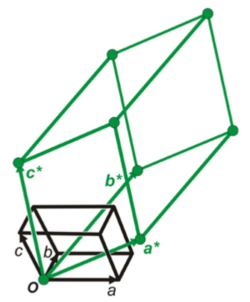
Alternative convention

Warning: In many areas of physics and in the context of matrix representations of point and space groups, the reciprocal basis is often scaled by a factor 2π:

$$\begin{pmatrix} \mathbf{a}\cdot\mathbf{a}^* & \mathbf{a}\cdot\mathbf{b}^* & \mathbf{a}\cdot\mathbf{c}^* \\ \mathbf{b}\cdot\mathbf{a}^* & \mathbf{b}\cdot\mathbf{b}^* & \mathbf{b}\cdot\mathbf{c}^* \\ \mathbf{c}\cdot\mathbf{a}^* & \mathbf{c}\cdot\mathbf{b}^* & \mathbf{c}\cdot\mathbf{c}^* \end{pmatrix} = \begin{pmatrix} 2\pi & 0 & 0 \\ 0 & 2\pi & 0 \\ 0 & 0 & 2\pi \end{pmatrix}$$

This simplifies the expression in the Fourier transform to $e^{i\mathbf{v}\cdot\mathbf{w}^*}$.

Properties of the reciprocal lattice



- $\mathbf{a}^*$ is perpendicular to the plane spanned by $\mathbf{b}$ and $\mathbf{c}$ and its projection to the line along $\mathbf{a}$ has length $1/|\mathbf{a}|$ (analogously for $\mathbf{b}^*$ and $\mathbf{c}^*$).
- If $\mathbf{a}, \mathbf{b}, \mathbf{c}$ span a unit cell of volume V, the reciprocal basis is given by vector products $\mathbf{a}^* = \frac{1}{V}(\mathbf{b} \times \mathbf{c})$, $\mathbf{b}^* = \frac{1}{V}(\mathbf{c} \times \mathbf{a})$, $\mathbf{c}^* = \frac{1}{V}(\mathbf{a} \times \mathbf{b})$.
- If $\mathbf{L}$ has metric tensor $\boldsymbol{G}$, then the metric tensor $\boldsymbol{G}^*$ of $\mathbf{L}^*$ is the inverse matrix $\boldsymbol{G}^* = \boldsymbol{G}^{-1}$.
- $(\mathbf{L}^*)^* = \mathbf{L}$.

Exercise

Let

$$\mathbf{a} = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

be the lattice basis of a (monoclinic) lattice $\mathbf{L}$.

Determine the reciprocal basis $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$.

Answer

By ones favourite method (direct inspection, vector product, ...) one finds

$$\mathbf{a}^* = \frac{1}{3}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{b}^* = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{c}^* = \frac{1}{3}\begin{pmatrix} -1 \\ 0 \\ 2 \end{pmatrix}$$

Exercise

Show that the reciprocal lattice of a body-centred cubic (bcc) lattice is a face-centred cubic (fcc) lattice (and vice-versa).
What is the relation between the cell parameters (for conventional cubic bases)?

Answer

- first assume cell parameter $a = 1$
- the bcc lattice $\mathbf{L}$ is spanned by $(1, 0, 0)$, $(0, 1, 0)$, $(0, 0, 1)$ and the centring vector $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$
- the vectors $\mathbf{w}^* \in \mathbf{L}^*$ have $\mathbf{v} \cdot \mathbf{w}^* \in \mathbb{Z}$ and are of the form (l, m, n) with $l + m + n$ even
- $\mathbf{L}^*$ is spanned by $(2, 0, 0)$, $(0, 2, 0)$, $(0, 0, 2)$ and the centring vectors $(1, 1, 0)$, $(1, 0, 1)$, $(0, 1, 1)$, this is an fcc lattice with cell parameter 2
- in the general case, $\mathbf{L}^*$ has cell parameter $\frac{2}{a}$
- the opposite direction follows, since $(\mathbf{L}^*)^* = \mathbf{L}$, note that $2/\frac{2}{a} = a$

The structure of space groups

Space group operations

- Space group operations are affine mappings, and can, with respect to a chosen coordinate system, be represented by a matrix-column pair $(\mathbf{W}, \mathbf{w})$.
- $\mathbf{W}$ is an invertible 3×3-matrix, called the linear part and $\mathbf{w}$ is a column, called the translation part of $(\mathbf{W}, \mathbf{w})$.
- $(\mathbf{W}, \mathbf{w})$ maps a point with coordinate column $\mathbf{x}$ to $\mathbf{W}\mathbf{x} + \mathbf{w}$.
- Since $\mathbf{W}\mathbf{o} = \mathbf{o}$, $\mathbf{w}$ is the translation of the origin $\mathbf{o}$ under $(\mathbf{W}, \mathbf{w})$.
- Translations are of the form $(\mathbf{I}, \mathbf{t})$ for $\mathbf{I}$ the 3×3-identity matrix.

Translation subgroup of a space group $\mathcal{G}$

- $\mathcal{T} = \{(\mathbf{I}, \mathbf{t}) \in \mathcal{G}\}$ is called the translation subgroup of $\mathcal{G}$
- $\mathbf{L} = \{\mathbf{t} \mid (\mathbf{I}, \mathbf{t}) \in \mathcal{G}\}$ is called the (translation) lattice of $\mathcal{G}$

Composition and inversion of matrix-column pairs

Composition

- Let $\mathbf{x}$ be the coordinate column of a point.
- $(\mathbf{W}_1, \mathbf{w}_1)$ maps $\mathbf{x}$ to $\mathbf{x}' = \mathbf{W}_1\mathbf{x} + \mathbf{w}_1$
- A further matrix-column pair $(\mathbf{W}_2, \mathbf{w}_2)$ maps the mapped point $\mathbf{x}'$ to

$$\mathbf{W}_2\mathbf{x}' + \mathbf{w}_2 = \mathbf{W}_2(\mathbf{W}_1\mathbf{x} + \mathbf{w}_1) + \mathbf{w}_2 = \underbrace{(\mathbf{W}_2\mathbf{W}_1)}_{\text{linear part}}\mathbf{x} + \underbrace{\mathbf{W}_2\mathbf{w}_1 + \mathbf{w}_2}_{\text{translation part}}.$$

- This shows that the composition $(\mathbf{W}_2, \mathbf{w}_2)(\mathbf{W}_1, \mathbf{w}_1)$ has the matrix-column pair

$$(\mathbf{W}_2\mathbf{W}_1, \mathbf{W}_2\mathbf{w}_1 + \mathbf{w}_2).$$

Question

Given the formula

$$(\mathbf{W}_2, \mathbf{w}_2)(\mathbf{W}_1, \mathbf{w}_1) = (\mathbf{W}_2\mathbf{W}_1, \mathbf{W}_2\mathbf{w}_1 + \mathbf{w}_2)$$

for composition just derived, can you work out a formula for the matrix-column pair of the inverse $(\mathbf{W}, \mathbf{w})^{-1}$ of $(\mathbf{W}, \mathbf{w})$?

Yes!

- Assume that $(\mathbf{W}', \mathbf{w}')$ is the inverse $(\mathbf{W}, \mathbf{w})^{-1}$.
- By the composition formula, $(\mathbf{W}'\mathbf{W}, \mathbf{W}'\mathbf{w} + \mathbf{w}')$ must be equal to the matrix-column pair $(\mathbf{I}, \mathbf{o})$ of the identity element.
- Comparing the linear parts shows that $\mathbf{W}' = \mathbf{W}^{-1}$.
- Inserting this in the translation part shows that $\mathbf{W}^{-1}\mathbf{w} + \mathbf{w}' = \mathbf{o}$, hence $\mathbf{w}' = -\mathbf{W}^{-1}\mathbf{w}$.
- Conclusion:
$$(\mathbf{W}, \mathbf{w})^{-1} = (\mathbf{W}^{-1}, -\mathbf{W}^{-1}\mathbf{w}).$$

Point group of a space group $\mathcal{G}$

- Composition $(\mathbf{W}_2, \mathbf{w}_2)(\mathbf{W}_1, \mathbf{w}_1) = (\mathbf{W}_2\mathbf{W}_1, \mathbf{W}_2\mathbf{w}_1 + \mathbf{w}_2)$ and inversion $(\mathbf{W}, \mathbf{w})^{-1} = (\mathbf{W}^{-1}, -\mathbf{W}^{-1}\mathbf{w})$
  show that the linear parts in $\mathcal{G}$ form a group by themselves
- $\mathcal{P} = \{\mathbf{W} \mid (\mathbf{W}, \mathbf{w}) \in \mathcal{G} \text{ for some } \mathbf{w}\}$ is called the point group of $\mathcal{G}$.

Interplay between point group and translation subgroup

- The computation of the conjugation

  $$\begin{aligned}(\mathbf{W},\, \mathbf{w})(\mathbf{I},\, \mathbf{t})(\mathbf{W},\, \mathbf{w})^{-1} &= (\mathbf{W},\, \mathbf{W}\mathbf{t} + \mathbf{w})(\mathbf{W}^{-1},\, -\mathbf{W}^{-1}\mathbf{w}) \\ &= (\mathbf{I},\, -\mathbf{w} + \mathbf{W}\mathbf{t} + \mathbf{w}) = (\mathbf{I},\, \mathbf{W}\mathbf{t})\end{aligned}$$

  has two important implications:
  - $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, since $(\mathbf{I},\, \mathbf{W}\mathbf{t})$ is again a translation.
  - The point group $\mathcal{P}$ acts on the translation lattice $\mathbf{L}$ of $\mathcal{G}$, since $(\mathbf{I},\, \mathbf{W}\mathbf{t}) \in \mathcal{T}$ implies $\mathbf{W}\mathbf{t} \in \mathbf{L}$ for $\mathbf{t} \in \mathbf{L}$.

The Bravais group of a lattice

- A point group operation $\mathbf{W}$ is an isometry that acts on $\mathbf{L}$.
- In particular, the scalar product is preserved by $\mathbf{W}$, i.e. $(\mathbf{Wv}) \cdot (\mathbf{Wv}') = \mathbf{v} \cdot \mathbf{v}'$
  $\Rightarrow$ $\mathbf{W}$ maps a lattice basis $\mathbf{a}, \mathbf{b}, \mathbf{c}$ to a new lattice basis $\mathbf{a}', \mathbf{b}', \mathbf{c}'$ with the same scalar products
  $\Rightarrow$ the metric tensor $\boldsymbol{G}$ is invariant under transformation by $\mathbf{W}$: $\mathbf{W}^{\mathsf{T}} \cdot \boldsymbol{G} \cdot \mathbf{W} = \boldsymbol{G}$.
- The full symmetry group $\mathcal{B} = \{\mathbf{W} \in \mathrm{GL}_3(\mathbb{Z}) \mid \mathbf{W}^{\mathsf{T}} \cdot \boldsymbol{G} \cdot \mathbf{W} = \boldsymbol{G}\}$ of a lattice $\mathbf{L}$ with metric tensor $\boldsymbol{G}$ is called the Bravais group of $\mathbf{L}$.
- $\mathcal{B}$ is finite, since its elements are determined by their action on a finite set of vectors.

Point groups are finite

The point group $\mathcal{P}$ of a space group $\mathcal{G}$ is a subgroup of the Bravais group of the lattice $\mathbf{L}$ of $\mathcal{G}$, in particular it is a finite group.

Overview of Bravais groups

Primitive lattices

lattice	$\mathcal{B}$	group symbol
triclinic	$\langle\bar{1}\rangle$	$\bar{1}$
monoclinic	$\langle\bar{1}, 2_{010}\rangle$	$2/m$
orthorhombic	$\langle m_{100}, m_{010}, m_{001}\rangle$	mmm
tetragonal	$\langle\bar{1}, 4^+_{001}, m_{100}\rangle$	$4/mmm$
hexagonal	$\langle\bar{1}, 6^+_{001}, m_{100}\rangle$	$6/mmm$
cubic	$\langle\bar{1}, 3^+_{111}, 4^+_{001}, m_{100}\rangle$	$m\bar{3}m$

Centred lattices

- Rhombohedral lattice: $\mathcal{B} = \langle\bar{3}^+_{111}, m_{1\bar{1}0}\rangle = \bar{3}m$
- For all other centred lattices, the Bravais group is conjugate to the Bravais group of the corresponding primitive lattice.

Coset decomposition with respect to $\mathcal{T}$

Right cosets relative to $\mathcal{T}$

- Left and right cosets of $\mathcal{G}$ relative to $\mathcal{T}$ are the same, since $\mathcal{T}$ is a normal subgroup of $\mathcal{G}$, but here it is more convenient to work with right cosets.
- For an element $(\mathbf{W}, \mathbf{w}) \in \mathcal{G}$ and $(\mathbf{I}, \mathbf{t}) \in \mathcal{T}$, we have $(\mathbf{I}, \mathbf{t})(\mathbf{W}, \mathbf{w}) = (\mathbf{W}, \mathbf{w} + \mathbf{t})$
  $\Rightarrow$ the right coset $\mathcal{T}(\mathbf{W}, \mathbf{w})$ with representative $(\mathbf{W}, \mathbf{w})$ consists of the elements with the same linear part $\mathbf{W}$ and with translation parts differing by lattice vectors from $\mathbf{L}$.
- Elements in different cosets have different linear parts
  $\Rightarrow$ in a system of coset representatives, every element from the point group $\mathcal{P}$ of $\mathcal{G}$ has to occur precisely once as linear part.
- $\mathcal{P} = \{\mathbf{W}_1, \ldots, \mathbf{W}_m\} \Rightarrow (\mathbf{W}_1, \mathbf{w}_1), \ldots, (\mathbf{W}_m, \mathbf{w}_m) \in \mathcal{G}$ is a system of coset representatives and
  $$\mathcal{G} = \mathcal{T}(\mathbf{W}_1, \mathbf{w}_1) \cup \ldots \cup \mathcal{T}(\mathbf{W}_m, \mathbf{w}_m)$$
  is the coset decomposition of $\mathcal{G}$ relative to $\mathcal{T}$.

Schematic view of the right-coset decomposition

$\mathcal{T}$	$\mathcal{T}(\mathbf{W}_2, \mathbf{w}_2)$	$\mathcal{T}(\mathbf{W}_3, \mathbf{w}_3)$	$\ldots$	$\mathcal{T}(\mathbf{W}_m, \mathbf{w}_m)$
$(\mathbf{I}, \mathbf{o})$	$(\mathbf{W}_2, \mathbf{w}_2)$	$(\mathbf{W}_3, \mathbf{w}_3)$	$\ldots$	$(\mathbf{W}_m, \mathbf{w}_m)$
$(\mathbf{I}, \mathbf{t}_2)$	$(\mathbf{W}_2, \mathbf{w}_2 + \mathbf{t}_2)$	$(\mathbf{W}_3, \mathbf{w}_3 + \mathbf{t}_2)$	$\ldots$	$(\mathbf{W}_m, \mathbf{w}_m + \mathbf{t}_2)$
$(\mathbf{I}, \mathbf{t}_3)$	$(\mathbf{W}_2, \mathbf{w}_2 + \mathbf{t}_3)$	$(\mathbf{W}_3, \mathbf{w}_3 + \mathbf{t}_3)$	$\ldots$	$(\mathbf{W}_m, \mathbf{w}_m + \mathbf{t}_3)$
$(\mathbf{I}, \mathbf{t}_4)$	$(\mathbf{W}_2, \mathbf{w}_2 + \mathbf{t}_4)$	$(\mathbf{W}_3, \mathbf{w}_3 + \mathbf{t}_4)$	$\ldots$	$(\mathbf{W}_m, \mathbf{w}_m + \mathbf{t}_4)$
$\vdots$	$\vdots$	$\vdots$		$\vdots$

Conventions for coset representatives

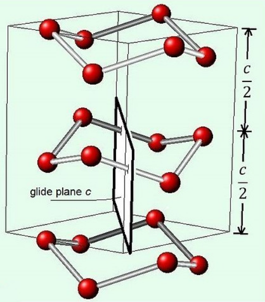
- With respect to a primitive basis of $\mathbf{L}$, the coordinate columns $\mathbf{t}$ for elements in $\mathbf{L}$ are simply the integral columns in $\mathbb{Z}^3$.
- There is a unique column $\mathbf{t} \in \mathbf{L}$ such that $\mathbf{w} + \mathbf{t}$ has all coordinates between 0 and 1, excluding 1
- It is customary to choose the coset representatives $(\mathbf{W}, \mathbf{w})$ such that their translation parts $\mathbf{w}$ have all their coordinates between 0 and 1, excluding 1.
- In particular, $\mathcal{T}(\mathbf{W}, \mathbf{w})$ has coset representative $(\mathbf{W}, \mathbf{o})$ if $\mathbf{w} \in \mathbf{L}$.

Glide reflections and screw rotations

Glide reflection in 2D

- reflection composed with translation along the mirror line
- composition with itself is a pure translation
  $\Rightarrow$ translation component is half of a lattice translation

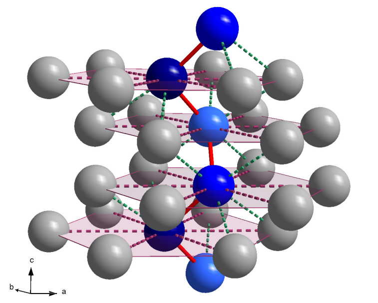
Glide reflection in 3D



- reflection composed with translation in the mirror plane
- matrix-column pair for example of glide reflection in ice:

$$\left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} \right)$$

Screw rotation



- rotation composed with translation along the rotation axis
- matrix-column pair for example of 3-fold screw rotation:

$$\left(\begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}\right)$$

Problem

Distinguishing glide reflections from ordinary reflections and screw rotations from ordinary rotations is obscured when the origin does not lie on the mirror plane or rotation axis.

Determining the type of a symmetry operation

Linear part: from determinant and trace

- determinant and trace (sum over diagonal entries) are invariant under basis transformations
- rotation $\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$ has trace $2\cos\theta + 1$
- rotoinversion $\begin{pmatrix} -\cos\theta & \sin\theta & 0 \\ -\sin\theta & -\cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix}$ has trace $-2\cos\theta - 1$
- inversion $\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ has trace -3
- reflection $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ has trace 1

Summary

type	proper rotations					improper rotations				
	1	2	3	4	6	$\bar{1}$	$\bar{3}$	$\bar{4}$	$\bar{6}$	$m = \bar{2}$
$\det \mathbf{W}$	1	1	1	1	1	-1	-1	-1	-1	-1
trace $\mathbf{W}$	3	-1	0	1	2	-3	0	-1	-2	1

Quick quiz

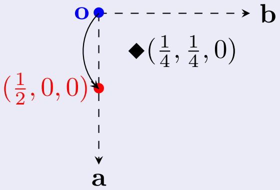
What types of point group operations are given by the matrices

$$\text{a)} \begin{pmatrix} 0 & -1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad \text{b)} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix}?$$

Answer

a) 6-fold rotoinversion $\bar{6}$, b) 2-fold rotation 2.

Example: 4-fold rotation around axis off the origin



- Although this is an ordinary 4-fold rotation, the matrix-column pair

$$\left(\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix} \right)$$

seems to indicate a screw rotation, since the translation part is nonzero.

Intrinsic translation part

- For $(\mathbf{W}, \mathbf{w})$ with $\mathbf{W}$ of order k, the k-th power $(\mathbf{W}, \mathbf{w})^k$ is a translation $(\mathbf{I}, \mathbf{t})$.
- The translation vector $\mathbf{w}_g = \frac{1}{k}\mathbf{t}$ is called the intrinsic translation part of $(\mathbf{W}, \mathbf{w})$.
- The remainder $\mathbf{w}_l = \mathbf{w} - \mathbf{w}_g$ is called the location part of $\mathbf{w}$.
- The intrinsic translation part $\mathbf{w}_g$ is always zero for inversions and rotoinversions, it lies in the mirror plane or rotation axis for $\mathbf{W}$ a reflection or rotation.
- The location part $\mathbf{w}_l$ is nonzero if the origin $\mathbf{o}$ does not lie on the geometric element (plane, axis), it can be transformed to zero by moving the origin appropriately.
- Removing the intrinsic translation by changing the translation part from $\mathbf{w}$ to the location part $\mathbf{w}_l$ gives an operation $(\mathbf{W}, \mathbf{w}_l)$ of finite order (rotation, reflection, inversion or rotoinversion).
- A point fixed by $(\mathbf{W}, \mathbf{w}_l)$ specifies the location of the geometric element of $(\mathbf{W}, \mathbf{w})$.

Example

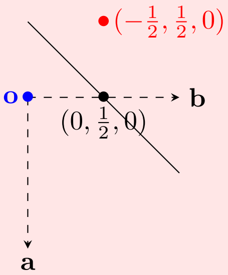
- What kind of symmetry operation is given by the matrix-column pair $(\mathbf{W},\mathbf{w}) = \left(\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ 0 \\ \frac{1}{2} \end{pmatrix}\right)$?
- linear part $\mathbf{W}$ is the 4-fold rotation 4^{+}_{001}
- $(\mathbf{W},\mathbf{w})^4 = \left(\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}\right)$
- intrinsic translation part is $\mathbf{w}_g = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}$, location part $\mathbf{w}_l = \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix}$
- $(\mathbf{W},\mathbf{w}_l)\mathbf{x} = \mathbf{x}$: $\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} \frac{1}{2} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -y + \frac{1}{2} \\ x \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$
  implies $-y + \frac{1}{2} = x$, $x = y$ and z arbitrary, thus $x = y = \frac{1}{4}$
- $(\mathbf{W},\mathbf{w})$ is a 4-fold screw rotation with screw translation $\frac{1}{2}\mathbf{c}$ and axis $(\frac{1}{4}, \frac{1}{4}, z)$

Exercise

What kind of symmetry operation is given by

$$(\mathbf{W}, \mathbf{w}) = \left(\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right)?$$

Hint:



Answer

- linear part $\mathbf{W}$ is the 2-fold rotation 2_{110}
- $(\mathbf{W},\mathbf{w})^2 = \left(\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix}, \begin{pmatrix}1\\ 1\\ 0\end{pmatrix}\right)$
- intrinsic translation part $\mathbf{w}_g = \begin{pmatrix}\frac{1}{2}\\ \frac{1}{2}\\ 0\end{pmatrix}$, location part $\mathbf{w}_l = \begin{pmatrix}-\frac{1}{2}\\ \frac{1}{2}\\ 0\end{pmatrix}$
- $(\mathbf{W},\mathbf{w}_l)\mathbf{x} = \mathbf{x}$: $\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix} + \begin{pmatrix}-\frac{1}{2}\\ \frac{1}{2}\\ 0\end{pmatrix} = \begin{pmatrix}y-\frac{1}{2}\\ x+\frac{1}{2}\\ z\end{pmatrix} = \begin{pmatrix}x\\ y\\ z\end{pmatrix}$
  implies $y - \frac{1}{2} = x$ and $z = 0$, the fixed points are $(x, x+\frac{1}{2}, 0)$
- $\Rightarrow (\mathbf{W},\mathbf{w})$ is a 2-fold screw rotation with screw translation $\frac{1}{2}(\mathbf{a}+\mathbf{b})$ and axis $(x, x+\frac{1}{2}, 0)$

Site-symmetry groups in space groups

Definition

The stabilizer of a point X under the action of a space group $\mathcal{G}$ is called its site-symmetry group, denoted by $\mathcal{S}_X$.

Remarks

- Site-symmetry groups can not contains translations, thus $\mathcal{S}_X$ contains at most one element from each coset relative to the translation subgroup $\mathcal{T}$ of $\mathcal{G}$.
- All elements in $\mathcal{S}_X$ have different linear parts and these linear parts form a subgroup of the point group $\mathcal{P}$ of $\mathcal{G}$.

Symmorphic and non-symmorphic space groups

Definition

If for some point X, $\mathcal{S}_X$ contains all linear parts from $\mathcal{P}$ and thus $|\mathcal{S}_X| = |\mathcal{P}|$, $\mathcal{G}$ is called a symmorphic space group.
Otherwise, $\mathcal{G}$ is called a non-symmorphic space group.

Alternative characterization

- Choosing a point X with $|\mathcal{S}_X| = |\mathcal{P}|$ as origin, the translation parts of the elements in $\mathcal{S}_X$ become all zero.
- Thus, after choosing an appropriate origin for a symmorphic space group, every coset relative to the translation subgroup $\mathcal{T}$ contains an element $(\mathbf{W}, \mathbf{o})$ with zero translation part.
- In a non-symmorphic space group $\mathcal{G}$, one or more of the coset representatives relative to $\mathcal{T}$ have non-trivial intrinsic translation part $\mathbf{w}_g$ (i.e. $\mathbf{w}_g \notin \mathbf{L}$).

Construction of symmorphic space groups

Canoncial assignment from an arbitrary space group

- For $\mathcal{G}$ with translation subgroup $\mathcal{T}$ and coset representatives $(\mathbf{W}_1, \mathbf{w}_1), \ldots, (\mathbf{W}_m, \mathbf{w}_m)$, change all translation parts in the coset representatives to $\mathbf{o}$.
- The space group $\mathcal{G}_0$ generated by $(\mathbf{W}_1, \mathbf{o}), \ldots, (\mathbf{W}_m, \mathbf{o})$ and $\mathcal{T}$ is a symmorphic space group with the same point group and translation subgroup as $\mathcal{G}$.

Construction from a lattice

- Let $\mathbf{L}$ be a lattice with Bravais group $\mathcal{B}$ and let $\mathcal{P}$ be a subgroup of $\mathcal{B}$.
- The space group $\mathcal{G} = \{(\mathbf{W}, \mathbf{w}) \mid \mathbf{W} \in \mathcal{P}, \mathbf{w} \in \mathbf{L}\}$ is a symmorphic space group in which the coset representatives can be chosen as $(\mathbf{W}, \mathbf{o})$.