Crystal Symmetry Primer*

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Contents

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0 Preliminary

This document gives an introduction to crystallography on crystal symmetry and space groups intended for computational materials science. We first consider group theoretic treatments of crystal symmetry in Secs. 1 and 2. Then, we analyze a group structure of space groups in Sec. 3, and the classification of space groups in Sec. 4. There are many conventions to take a representative among "equivalent" objects. We introduce some of the conventions to avoid pitfalls in Sec. 5. The remaining sections are potpourris. In Sec. 6, we consider a group structure of magnetic space groups and conventions to represent them. In Sec. 7, we introduce normalizers of space groups, useful to treat the arbitrariness of transformation. In Sec. 8, we consider standard forms of integer matrices, which can be applied to supercell constructions and generalized regular meshes for Brillouin zone sampling.

There are already many impressive books and lectures covering the topic:

- M. I. Aroyo, editor. *International Tables for Crystallography*, volume A. International Union of Crystallography, December 2016
- M I Aroyo. *Teaching edition of international tables for crystallography - crystallographic symmetry, sixth edition*. IUCr Series. International Tables for Crystallography. John Wiley & Sons, Nashville, TN, 6 edition, May 2021
- Bernd Souvignier. Group theory applied to crystallography. `https://www.math.ru.nl/~souvi/krist_09/cryst.pdf`
- Ulrich Müller. *Symmetry relationships between crystal structures: applications of crystallographic group theory in crystal chemistry*, volume 18. OUP Oxford, 2013
- Michael Glazer, Gerald Burns, and Alexander N Glazer. *Space groups for solid state scientists*. Elsevier, 2012
- Commission for Crystallographic Nomenclature of the International Union of Crystallography. Online dictionary of crystallography. `https://dictionary.iucr.org/Main_Page`

In Japanse,

- Yuji Tachikawa, 物理数学 III (2018)
- 対称性・群論トレーニングコース
- 野田幸男, 結晶学と構造物性 入門から応用、実践まで (内田老鶴圃, 2017)

If you find typos or errors, please open an issue or pull request.

1 Symmetry operation and space group

1.1 Affine group

1.1.1 Lattice

Definition 1.1 (lattice)**.** *Lattice* L in $\mathbb{R}^n$ is the set spanned by n independet vectors $\boldsymbol{a}_1, \dots, \boldsymbol{a}_n$ as

$$L \coloneqq \left\{ \sum_{i=1}^{n} l_i \boldsymbol{a}_i \;\middle|\; l_1, \dots, l_n \in \mathbb{Z} \right\}. \tag{1}$$

These vectors $\boldsymbol{a}_1, \dots, \boldsymbol{a}_n$ are called *lattice basis* of L.

We introduce the standard inner product in vector space $\mathbb{R}^n$. Then it is convenient to define the following matrix for calculating distances.

Definition 1.2 (metric tensor)**.** Let $\mathbf{A} \coloneqq (\mathbf{a}_1, \dots, \mathbf{a}_n)$ be basis vectors of a lattice L. A *metric tensor* of L is

$$\boldsymbol{G} \coloneqq \boldsymbol{A}^\top \boldsymbol{A}. \tag{2}$$

We remark that metric tensor $\boldsymbol{G}$ implicitly depends on the choice of basis vectors of L. When basis vectors are changed from $\boldsymbol{A}$ to $\boldsymbol{AP}$, the metric tensor are changed from $\boldsymbol{G} = \boldsymbol{A}^\top \boldsymbol{A}$ to $\boldsymbol{P}^\top \boldsymbol{GP}$.

Be careful basis vectors $\boldsymbol{A}$ are column-wise whereas programmers often use row-wise basis vectors.

```python
import numpy as np
# Row-wise basis vectors
lattice = np.array([
    [ax, ay, az],  # a axis
    [bx, by, bz],  # b axis
    [cx, cy, cz],  # c axis
])
# Fractional coordiantes
frac_coords = np.array([
    [p0, q0, r0],
    [p1, q1, r1],
    ...
])
# Cartesian coordinates
cart_coords = np.dot(frac_coords, lattice)
```

1.1.2 Affine mapping

To display components of points, we fix some orgin O and basis $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$ in $\mathbb{R}^n$. We define *affine space* by using O and $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$.

$$\mathbb{A}_n := \left\{ \begin{pmatrix} x_1 \\ \vdots \\ x_n \\ 1 \end{pmatrix} \middle| \; x_1 \ldots, x_n \in \mathbb{R} \right\}. \tag{3}$$

Here, $(0, \ldots, 0, 1)^\top \in \mathbb{A}_n$ corresponds to the origin O, and the ith components x_i corresponds to the basis $\boldsymbol{a}_i$.

Definition 1.3 (affine group)**.** An *affine mapping* $\begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \mathbf{0}^\top & 1 \end{pmatrix}$ ($\boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \boldsymbol{w} \in \mathbb{R}^n$)[a] is a mapping that moves a point $\begin{pmatrix} \boldsymbol{x} \\ 1 \end{pmatrix} \in \mathbb{A}_n$ to

$$\begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \mathbf{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{x} \\ 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} \\ 1 \end{pmatrix} \in \mathbb{A}_n. \tag{4}$$

The matrix $\boldsymbol{W}$ is called the *linear part* and the vector w is called the *translation part*.
The *affine group* $\mathcal{A}_n$ is the set of affine mappings

$$\mathcal{A}_n := \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \mathbf{0}^\top & 1 \end{pmatrix} \middle| \; \boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{5}$$

[a] The general linear group $\mathrm{GL}(n, \mathbb{R})$ is the set of $n \times n$ invertible real matrices.

We often identify a point $\begin{pmatrix} \boldsymbol{x} \\ 1 \end{pmatrix} \in \mathbb{A}_n$ as $\boldsymbol{x} \in \mathbf{R}^n$ and write an affine mapping $\begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \mathbf{0}^\top & 1 \end{pmatrix}$ as $(\boldsymbol{W}, \boldsymbol{w})$ or $\{\boldsymbol{W} \mid \boldsymbol{w}\}$. Then the action of the affine mapping is compactly written as

$$(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} := \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} \tag{6}$$

$$\{\boldsymbol{W} \mid \boldsymbol{w}\}\boldsymbol{x} := \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} \tag{7}$$

The notation for affine mapping in Eq. (6) is called *matrix-column pair*, and the one in Eq. (7) is called *Seitz symbol*[1]. The original $(n+1) \times (n+1)$ matrix is also called an *augmented matrix*[2].

[1] Do not write $(\boldsymbol{W} \mid \boldsymbol{w})$ or $\{\boldsymbol{W}, \boldsymbol{w}\}$!

[2] The augmented matrix is a 4×4 matrix in three dimensions. Because the fourth column is always constant, the column is often omitted in computer vision.

1.1.3 Combination and inverse of affine mappings

Consider two affine mappings $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$. Then $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ maps $\boldsymbol{x}$ to $\boldsymbol{x}'$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ maps $\boldsymbol{x}'$ to $\boldsymbol{x}''$. We define a combination of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ and $(\boldsymbol{W}_2, \boldsymbol{w}_2)$ so that it maps $\boldsymbol{x}$ to $\boldsymbol{x}''$,

$$\begin{aligned}
\boldsymbol{x}' &= (\boldsymbol{W}_1, \boldsymbol{w}_1)\boldsymbol{x} = \boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{w}_1 \\
\boldsymbol{x}'' &= (\boldsymbol{W}_2, \boldsymbol{w}_2)\boldsymbol{x}' = \boldsymbol{W}_2\boldsymbol{x}' + \boldsymbol{w}_2 \\
&= \boldsymbol{W}_2\boldsymbol{W}_1\boldsymbol{x} + \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2
\end{aligned}$$

$$\therefore \quad (\boldsymbol{W}_2, \boldsymbol{w}_2)(\boldsymbol{W}_1, \boldsymbol{w}_1) \coloneqq (\boldsymbol{W}_2\boldsymbol{W}_1, \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2). \tag{8}$$

We define an inverse of $(\boldsymbol{W}_1, \boldsymbol{w}_1)$ so that it maps $\boldsymbol{x}'$ to $\boldsymbol{x}$,

$$\boldsymbol{x} = \boldsymbol{W}_1^{-1}\boldsymbol{x}' - \boldsymbol{W}_1^{-1}\boldsymbol{w}_1$$

$$\therefore \quad (\boldsymbol{W}_1, \boldsymbol{w}_1)^{-1} \coloneqq (\boldsymbol{W}_1^{-1}, -\boldsymbol{W}_1^{-1}\boldsymbol{w}_1). \tag{9}$$

These computations can be written as usual matrix operations,

$$\begin{pmatrix} \boldsymbol{W}_2 & \boldsymbol{w}_2 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}_2\boldsymbol{W}_1 & \boldsymbol{W}_2\boldsymbol{w}_1 + \boldsymbol{w}_2 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \tag{10}$$

$$\begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix}^{-1} = \begin{pmatrix} \boldsymbol{W}_1^{-1} & -\boldsymbol{W}_1^{-1}\boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix}^{-1}. \tag{11}$$

1.1.4 short-hand notation

The matrix-column pair $(\boldsymbol{W}, \boldsymbol{w})$ is often represented in the *short-hand notation*, which consists of a tuple

$$W_{11}x + W_{12}y + W_{13}z, W_{21}x + W_{22}y + W_{23}z, W_{31}x + W_{32}y + W_{33}z.$$

The coefficients "+1" are omitted. The terms with the "0" coefficient are also omitted. The negative term $-x$ is replaced with $\overline{x}$.

Note that we implicitly take the basis of $(\boldsymbol{W}, \boldsymbol{w})$ such that $\boldsymbol{W}$ is an integer matrix. For example, let $\boldsymbol{e}_x$ and $\boldsymbol{e}_y$ be a standard basis of $\mathbb{R}^2$. The rotation with angle $\frac{2\pi}{3}$ acts on the basis as

$$\hat{R}_{\frac{2\pi}{3}}(\boldsymbol{e}_x\, \boldsymbol{e}_y) = (\boldsymbol{e}_x\, \boldsymbol{e}_y) \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}.$$

If we take the hexagonal axis

$$(\boldsymbol{e}_1\, \boldsymbol{e}_2) = (\boldsymbol{e}_x\, \boldsymbol{e}_y) \begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix},$$

the rotation $\hat{R}_{2\frac{\pi}{3}}$ is represented as an integer matrix,

$$
\begin{aligned}
\hat{R}_{\frac{2\pi}{3}}(\boldsymbol{e}_1\,\boldsymbol{e}_2) &= (\boldsymbol{e}_1\,\boldsymbol{e}_2)\begin{pmatrix}1 & -\frac{1}{2}\\ 0 & \frac{\sqrt{3}}{2}\end{pmatrix}^{-1}\begin{pmatrix}-\frac{1}{2} & -\frac{\sqrt{3}}{2}\\ \frac{\sqrt{3}}{2} & -\frac{1}{2}\end{pmatrix}\begin{pmatrix}1 & -\frac{1}{2}\\ 0 & \frac{\sqrt{3}}{2}\end{pmatrix}\\
&= (\boldsymbol{e}_1\,\boldsymbol{e}_2)\begin{pmatrix}0 & -1\\ 1 & -1\end{pmatrix}.
\end{aligned}
$$

The coordinates tuple $\overline{x}, x-y$ represents this rotation.

1.1.5 Transformation matrix and origin shift

When we change the origin and basis vectors for the affine space from O and $\boldsymbol{A} = (\boldsymbol{a}_1, \dots, \boldsymbol{a}_3)$ to $\boldsymbol{A}\boldsymbol{p}$ and $(\boldsymbol{a}_1, \dots, \boldsymbol{a}_3)\boldsymbol{P}$, the components of point coordinates and affine mappings are also changed as follows.

The point coordinates $\boldsymbol{x}$ is transformed to the new coordinates $\boldsymbol{x}'$

$$
\begin{aligned}
\boldsymbol{x}' &= (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x}\\
&= \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p}).
\end{aligned}
\tag{12}
$$

An affine mapping $(\boldsymbol{W}, \boldsymbol{w})$ is transformed to $(\boldsymbol{W}', \boldsymbol{w}')$

$$
\begin{aligned}
(\boldsymbol{W}', \boldsymbol{w}') &= (\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})\\
&= \left(\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}, \boldsymbol{P}^{-1}(\boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p})\right).
\end{aligned}
\tag{13}
$$

The metric tensor $\boldsymbol{G}$ of the lattice spanned the basis vectors of the affine space is transformed to

$$
\boldsymbol{G}' = \boldsymbol{P}^\top \boldsymbol{G}\boldsymbol{P}. \tag{14}
$$

1.2 Euclidean group

Definition 1.4 (isometry)**.** Let $\boldsymbol{G}$ be a metric tensor. An affine mapping $(\boldsymbol{W}, \boldsymbol{w})$ is called *isometry* if $\boldsymbol{W}^\top \boldsymbol{G}\boldsymbol{W} = \boldsymbol{G}$.

We remark that an isometry affine mapping does not change the distance between two points and vice versa.

$$
\begin{aligned}
&\forall \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n, \|\boldsymbol{A}(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x} - \boldsymbol{A}(\boldsymbol{W}, \boldsymbol{w})\boldsymbol{y}\| = \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{A}\boldsymbol{y}\|\\
&\iff \forall \boldsymbol{x} \in \mathbb{R}^n, \|\boldsymbol{A}\boldsymbol{W}\boldsymbol{x}\| = \|\boldsymbol{A}\boldsymbol{x}\|\\
&\iff \boldsymbol{A}\boldsymbol{W}\boldsymbol{A}^{-1} \text{ is orthogonal}\\
&\iff \boldsymbol{W}^\top \boldsymbol{G}\boldsymbol{W} = \boldsymbol{G}
\end{aligned}
$$

Definition 1.5 (Euclidean group)**.** The *Euclidean group* $\mathcal{E}_n$ is the set of isometry affine mappings

$$\mathcal{E}_n := \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \middle| \boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G}, \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{15}$$

Definition 1.6 (Translation subgroup)**.** The *translation subgroup* of $\mathcal{A}_n$ is the set of affine mappings whose linear parts are identity,

$$\mathcal{T}_n := \left\{ \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \middle| \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{16}$$

1.3 Symmetry group

1.3.1 Symmetry operation and space group

A *symmetry operation* is an isometry affine mapping between two objects. For example, see Figs 4.1 and 4.2 of Ref. [4] for illustrations of symmetry operations in three dimensions.

Loosely speaking, a *space group* is a set of symmetry operations that preserve a three-dimensional crystal pattern. Similarly, a set of symmetry operations for a two-dimensional crystal pattern is called *plane group*. We consider a more rigorous definition of space groups in Sec. 3.1.

1.3.2 Working examples from plane groups

We introduce some plane groups in augmented matrices as working examples. These plane groups are shown in Fig. 1.

The plane group *pm* is generated by the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

which correspond to $t(1,0)$, $t(0,1)$, and m operations, respectively[3].

The plane group *cm* is generated by the matrices

$$\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & 1 & -\frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

[3] Do not worry about the notations for symmetry operations such as $t(1,0)$ or m_{10}. They are not required to read the remained document.

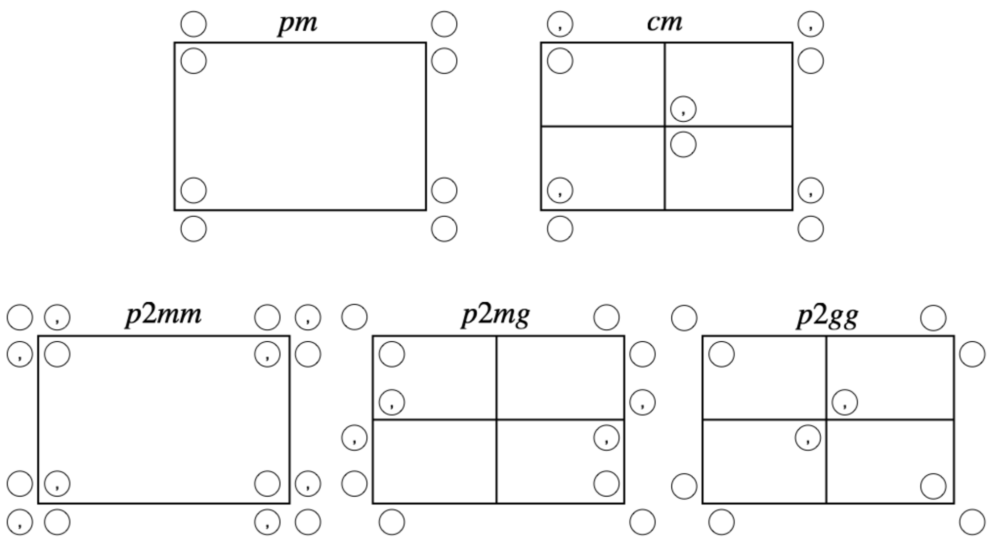

Figure 1: Example diagrams of plane groups

which correspond to $t(\frac{1}{2},\frac{1}{2})$, $t(\frac{1}{2},-\frac{1}{2})$, and m operations, respectively.

The plane group $p2mm$ is generated by the matrices,

$$\left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

which correspond to $t(1,0)$, $t(0,1)$, 2, m_{01}, and m_{10} operations, respectively.

The plane group $p2mg$ is generated by the matrices,

$$\left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right),$$

which correspond to $t(1,0)$, $t(0,1)$, 2, m, and a operations, respectively.

The plane group $p2gg$ is generated by the matrices,

$$\left(\begin{array}{cc|c} 1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} \\ 0 & -1 & \frac{1}{2} \\ \hline 0 & 0 & 1 \end{array}\right),$$

which correspond to $t(1,0)$, $t(0,1)$, 2, b, and a operations, respectively.

2 Group theory primer

You may be already familiar with group theory. If not so, the following textbooks are recommended as standard ones in the fields of physics and materials science.

- Mildred S Dresselhaus, Gene Dresselhaus, and Ado Jorio. *Group theory: application to the physics of condensed matter*. Springer-Verlag, Heidelberg, Berlin, 2010
- Michael El-Batanouny and Frederick Wooten. *Symmetry and condensed matter physics: a computational approach*. Cambridge University Press, Cambridge, UK, 2008
- Teturo Inui, Yukito Tanabe, and Yositaka Onodera. *Group theory and its applications in physics*. Springer Series in Solid-State Sciences. Springer, Berlin, Germany, March 1996

Here, we briefly prepare notations for group theory and introduce notions in crystallography in terms of group theory[4].

2.1 Definition

Definition 2.1 (group [10])**.** A *group* is a set G with a binary operation $\circ : G \times G \to G$ that satisfies the following properties:

- (Closure) For all $g, h \in G$, $g \circ h \in G$;
- (Associativity) For all $g, h, k \in G$, $(g \circ h) \circ k = g \circ (h \circ k)$;
- (Identity) There exists a unique element $e \in G$ satisfying $g \circ e = e \circ g = g$ for all $g \in G$;
- (Identity) For all $g \in G$, there exists an inverse of g, denoted by g^{-1} such that $g \circ g^{-1} = g^{-1} \circ g = e$.

If a group G is finite, the number of G is called the *order* of G, denoted by $|G|$. A subset of G is called *generators* if all elements in G can be written as a finite product of elements of the subset. We write the products of group elements as gh instead of $g \circ h$ as possible for conciseness.

We mention that the affine group $\mathcal{A}_n$ is group: For $\begin{pmatrix} \boldsymbol{W}_i & \boldsymbol{w}_i \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \in \mathcal{A}_n (i = 1, 2)$, the product of two affine mappings is also affine mapping,

$$\begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{W}_2 & \boldsymbol{w}_2 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}_1 \boldsymbol{W}_2 & \boldsymbol{W}_1 \boldsymbol{w}_2 + \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \in \mathcal{A}_n. \tag{17}$$

The associativity is followed by matrix multiplications. The identity $\begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{0} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}$ belongs to $\mathcal{A}_n$. The inverse of an affine mapping is also an affine mapping,

$$\begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}_1^{-1} & -\boldsymbol{W}_1^{-1} \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \in \mathcal{A}_n. \tag{18}$$

[4] We mainly adopt definitions in Refs. [1] and [10].

Definition 2.2 (Abeliean group)**.** A group G is called *Abelian* if $g \circ h = h \circ g$ for all $g, h \in G$.

A translation subgroup of $\mathcal{A}_n$ is an abelian group: for all $\boldsymbol{w}, \boldsymbol{w}' \in \mathbb{R}^n$,

$$\begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w}' \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w} + \boldsymbol{w}' \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w}' \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}.$$

2.2 Subgroup

Definition 2.3 (subgroup [10])**.** A subset H of a group G is called *subgroup* of G if it forms a group under the same operation as that of G.

The following criteria are commonly used to check a subset H of group G is a subgroup.

Proposition 2.4. A subset H of group G is a subgroup of G if and only if

- For all $h, h' \in H$, $hh' \in H$;
- and for all $h \in H$, $h^{-1} \in H$.

Proposition 2.5. A subset H of group G is a subgroup of G if and only if $h^{-1}h' \in H$ for all $h, h' \in H$.

The Euclidean group is a subgroup of the affine group. Let $\boldsymbol{G}$ be a metric tensor. For $(\boldsymbol{W}, \boldsymbol{w}), (\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{E}_n$, $\boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G}$ and $\boldsymbol{W}'^\top \boldsymbol{G} \boldsymbol{W}' = \boldsymbol{G}$. Then, $\boldsymbol{W}\boldsymbol{W}'$ gives an isometry affine mapping,

$$(\boldsymbol{W}\boldsymbol{W}')^\top \boldsymbol{G} (\boldsymbol{W}\boldsymbol{W}') = \boldsymbol{W}'^\top (\boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W}) \boldsymbol{W}' = \boldsymbol{W}'^\top \boldsymbol{G} \boldsymbol{W}' = \boldsymbol{G}.$$

Because $\boldsymbol{G}$ is symmetric, $\boldsymbol{W}\boldsymbol{G}\boldsymbol{W}^\top = \boldsymbol{G}$, which gives $\boldsymbol{G} = \boldsymbol{W}^{-\top} \boldsymbol{G} \boldsymbol{W}^{-1}$. Thus, $\boldsymbol{W}^{-1}$ also gives an isometry affine mapping.

2.3 Group action

2.3.1 Action

Definition 2.6 (action)**.** A *group action* of a group G on a set X is a mapping $\phi_g : X \to X$ for each $g \in G$ satisfying

- $\phi_{gh} = \phi_g \phi_h$ for all $g, h \in G$[a];
- $\phi_e(x) = x$ for all $x \in X$.

Then, we say that G *acts* on X.

[a]This means $\phi_{gh}(x) = \phi_g(\phi_h(x))$ for all $x \in X$.

We write $\phi_g(x)$ as gx in most cases.

The affine group $\mathcal{A}_n$ acts on the affine space $\mathbb{A}_n$. Rather, we define the operation of affine mappings to be group action in Sec. 1.1.3.

2.3.2 Orbit and crystallographic orbit

Definition 2.7 (orbit)**.** Let a group G act on a set X. Two elements $x, y \in X$ lie in the same *orbit* under G if there exists $g \in G$ such that $y = gx$. The set

$$G(x) \coloneqq \{gx \mid g \in G\} \tag{19}$$

is called the orbit of x under G.

Definition 2.8 (crystallographic orbit)**.** An orbit under a space group is called a *crystallographic orbit.*

The diagrams of plane groups in Fig. 1 can be seen as orbits of points under each plane group.

2.3.3 Stablilizer and site-symmetry group

Definition 2.9 (stabilizer)**.** Let a group G act on X. The *stabilizer* of $x \in X$ in G is

$$\mathrm{Stab}_G(x) \coloneqq \{g \in G \mid gx = x\}\,. \tag{20}$$

The stabilizer is a subgroup: for $g, h \in \mathrm{Stab}_G(x)$, $(g^{-1}h)x = g^{-1}(hx) = g^{-1}x = x$.

A space group acts on points in $\mathbb{R}^n$. We consider classifying the points with respect to the action of the space group.

Definition 2.10 (site-symmetry group)**.** The stabilizer of a point $\boldsymbol{x} \in \mathbb{R}^n$ on space group $\mathcal{G}$ is called *site-symmetry group* of $\boldsymbol{x}$.

Definition 2.11 (General and special positions)**.** A point $\boldsymbol{x} \in \mathbb{R}^n$ is called a point in a *general position* for a space group $\mathcal{G}$ if its site-symmetry group is identity. Otherwise, $\boldsymbol{x}$ is called a point in a *special position.*

Example: site-symmetry groups on pm The symmetry operations of pm are represented in augmented matrices as

$$\left(\begin{array}{cc|c} 1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where $t_1, t_2 \in \mathbb{Z}$. The fixed points of each symmetry operation are

- $\left(\begin{array}{cc|c} 1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: all points for $(t_1, t_2) = (0, 0)$, and nothing for otherwise;
- $\left(\begin{array}{cc|c} -1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: $(x, y) = (\frac{t_1}{2}, *)$ for $t_2 = 0$, and nothing for otherwise.

Thus, site-symmetry groups of points in $\{(x, y) \mid 0 \leq x < 1, 0 \leq y < 1\}$ are

$$\begin{aligned} (0, y) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\ \left(\frac{1}{2}, y\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\ \text{otherwise} &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\}. \end{aligned}$$

The points $(0, y)$ and $\left(\frac{1}{2}, y\right)$ are points in special positions.

Example: site-symmetry groups on $p2mg$ The symmetry operations of $p2mg$ are represented in augmented matrices as

$$\left(\begin{array}{cc|c} 1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & t_1 \\ 0 & -1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} + t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2} + t_1 \\ 0 & -1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right),$$

where $t_1, t_2 \in \mathbb{Z}$. The fixed points of each symmetry operation are

- $\left(\begin{array}{cc|c} 1 & 0 & t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: all points for $(t_1, t_2) = (0, 0)$, and nothing for otherwise;
- $\left(\begin{array}{cc|c} -1 & 0 & t_1 \\ 0 & -1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: $(x, y) = (\frac{t_1}{2}, \frac{t_2}{2})$;
- $\left(\begin{array}{cc|c} -1 & 0 & \frac{1}{2} + t_1 \\ 0 & 1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: $(x, y) = \left(\frac{t_1}{2} + \frac{1}{4}, *\right)$ for $t_2 = 0$, and nothing for otherwise;

- $\left(\begin{array}{cc|c} 1 & 0 & \frac{1}{2}+t_1 \\ 0 & -1 & t_2 \\ \hline 0 & 0 & 1 \end{array}\right)$: nothing.

Thus, site-symmetry groups of points in $\{(x,y) \mid 0 \leq x < 1, 0 \leq y < 1\}$ are

$$
\begin{aligned}
(0,0) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\left(\frac{1}{2},0\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & -1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\left(0,\frac{1}{2}\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\left(\frac{1}{2},\frac{1}{2}\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & -1 & 1 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\left(\frac{1}{4},y\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\left(\frac{3}{4},y\right) &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right), \left(\begin{array}{cc|c} -1 & 0 & 1 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\} \\
\text{otherwise} &: \left\{ \left(\begin{array}{cc|c} 1 & 0 & 0 \\ 0 & 1 & 0 \\ \hline 0 & 0 & 1 \end{array}\right) \right\}.
\end{aligned}
$$

The points $(0,0)$, $\left(\frac{1}{2},0\right)$, $\left(0,\frac{1}{2}\right)$, $\left(\frac{1}{2},\frac{1}{2}\right)$, $\left(\frac{1}{4},y\right)$, and $\left(\frac{3}{4},y\right)$ are points in special positions.

2.4 Isomorphism and conjugacy

2.4.1 Isomoprhism

Definition 2.12 (isomorphism)**.** Let G and H be groups. A bijection $\phi : G \to H$ is called *isomorphism* if $\phi(gg') = \phi(g)\phi(g')$ for all $g, g' \in G$. If an isomorphism exists between G and H, they are called *isomorphic* and denoted by $G \cong H$.

The translation subgroup of $\mathcal{A}_n$ is isomorphic to $\mathbb{R}^n$ by the bijection $\mathcal{T}_n \ni (\boldsymbol{I}_n, \boldsymbol{w}) \mapsto \boldsymbol{w} \in \mathbb{R}^n$.

2.4.2 Conjugacy subgroup and Wyckoff position

Let us classify subgroups of group G. First, we consider an action of G on G.

Definition 2.13 (conjugation)**.** Let G be a group. The action of G on G,

$$\bullet^g : G \ni h \mapsto h^g := g^{-1}hg \in G, \tag{21}$$

is called *conjugation*[a]. The orbits of the actions are called *conjugacy classes* of G. Elements in the same conjugacy class are called to be *conjugate* in G.

[a] Check $h^{gg'} = (h^g)^{g'}$.

The conjugation gives an equivalence relationship between subgroups.

Definition 2.14 (conjugate subgroup)**.** Let H be a subgroup of G. The set

$$H^g := g^{-1}Hg = \{h^g \mid h \in H\} \tag{22}$$

is an isomorphic subgroup to H, which called a *conjugate subgroup*.

Now, consider classifying points in special positions more finely. We observe each point in a crystallographic orbit under a space group $\mathcal{G}$ gives a conjugate subgroup to each other: for $\boldsymbol{x} = g\boldsymbol{y}$,

$$\begin{aligned} \mathrm{Stab}_{\mathcal{G}}(\boldsymbol{y}) &= \left\{ h \in G \,\middle|\, ghg^{-1}\boldsymbol{x} = \boldsymbol{x} \right\} \\ &= \left\{ g^{-1}hg \,\middle|\, h \in \mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x}) \right\} \\ &= g^{-1} \circ \mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x}) \circ g. \end{aligned} \tag{23}$$

The conjugate subgroups motivate the classification of site-symmetry groups by conjugations.

Definition 2.15 (Wyckoff position)**.** Two points $\boldsymbol{x}$ and $\boldsymbol{y}$ belong to the same *Wyckoff position* for a space group $\mathcal{G}$ if their site-symmetry groups are conjugate subgroups of $\mathcal{G}$.

Note that the Wyckoff position of $\boldsymbol{x}$ contains all the points in $\mathcal{G}(\boldsymbol{x})$. Also, two points in different orbits will belong to the same Wyckoff position. For example, all points in general positions belong to the same Wyckoff position.

If a point $\boldsymbol{x}$ has a different site-symmetry group than its neighbor, the points belonging to the Wyckoff position are identical to the orbit of $\boldsymbol{x}$. We can prove this by contradiction (see Fig. 2 for sketch of proof). Let $\boldsymbol{x}$ be a point with a different site-symmetry group than its neighbor. Suppose a point $\boldsymbol{y}$ has a conjugate subgroup $\mathrm{Stab}_{\mathcal{G}}(\boldsymbol{y}) = g^{-1}\mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x})g$, but $\boldsymbol{x}$ and $\boldsymbol{y}$ do not belong to the same crystallographic orbit. Then, the site-symmetry group of $\boldsymbol{y}' = g\boldsymbol{x}$ is $\mathrm{Stab}_{\mathcal{G}}(\boldsymbol{y}') = g\mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x})g^{-1} = \mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x})$.

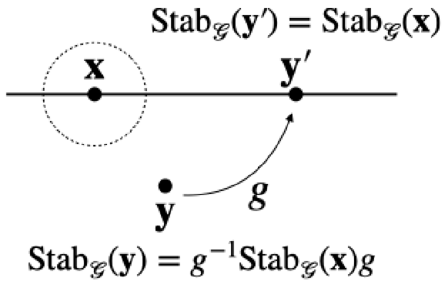

Figure 2: The Wyckoff position for an isolated point is identical to its crystallographic orbit.

Then, $\boldsymbol{x}$ and $\boldsymbol{y}'$ are different points by assumption. Because the points in a line connecting $\boldsymbol{x}$ and $\boldsymbol{y}'$ have the same site-symmetry group with $\mathrm{Stab}_{\mathcal{G}}(\boldsymbol{x})$, there is a neighbor point of $\boldsymbol{x}$ that has the same site-symmetry group with $\boldsymbol{x}$, which is a contradiction.

The Wyckoff positions are often displayed with *Wyckoff multiplicity* and *Wyckoff letter*. The Wyckoff multiplicity denotes the number of points in a crystallographic orbit lying in the conventional cell. The Wyckoff letter labels each Wyckoff position by a single letter starting from "a"[5].

Example: Wyckoff positions of pm

- $(0, y) \Rightarrow 1a$
- $\left(\frac{1}{2}, y\right) \Rightarrow 1b$
- otherwise $\Rightarrow 2c$

Example: Wyckoff positions of $p2mg$

- $(0,0), \left(\frac{1}{2}, 0\right) \Rightarrow 2a$
- $\left(0, \frac{1}{2}\right), \left(\frac{1}{2}, \frac{1}{2}\right) \Rightarrow 2b$
- $\left(\frac{1}{4}, y\right), \left(\frac{3}{4}, y\right) \Rightarrow 2c$
- otherwise $\Rightarrow 4d$

2.5 Coset, normal subgroup, and factor group

Definition 2.16 (coset)**.** Let H be a subgroup of G. For $g \in G$, the subset

$$gH \coloneqq \{gh \mid h \in H\} \tag{24}$$

is called the *left coset* of H with *representative* g.

[5] *Pmmm* (No. 47) has 27 Wyckoff positions. Thus, the Latin alphabet is not enough for Wyckoff letters.

The coset eH is H itself. Two cosets gH and $g'H$ are equal if and only if $g^{-1}g' \in H$. Otherwise, gH and $g'H$ are disjoint.

A group can be decomposed into disjointed cosets,

$$G = \bigsqcup_i g_i H. \tag{25}$$

Definition 2.17 (normal subgroup)**.** A subgroup N of group G is called *normal* if $N^g = N$ for all $g \in G$, denoted as $N \trianglelefteq G$.

The normal subgroup is characterized by the property that the product of any $gn \in gN$ and $g'n' \in g'N$ belongs to $gg'N$[6].

Definition 2.18 (factor group)**.** The *factor group* of group G by normal subgroup N is a set of cosets gN $(g \in G)$ with the binary operation, $gH \circ g'H = gg'H$.

The translation subgroup $\mathcal{T}_n$ is a normal subgroup of $\mathcal{A}_n$,

$$\begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{t} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{W}^{-1}(\boldsymbol{t} - \boldsymbol{w}) \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \in \mathcal{T}_n.$$

2.6 homomorphism, kernel, image

Definition 2.1 (homomorphism)**.** Let G and H be groups. A map $\phi : G \to H$ is called *homomorphism* if $\phi(gg') = \phi(g)\phi(g')$ for all $g, g' \in G$.

Definition 2.2 (kernel)**.** Let $\phi : G \to H$ be a homomorphism between groups G and H. The set

$$\mathrm{Ker}(\phi) := \{g \in G \mid \phi(g) = e\} \tag{26}$$

is called a *kernel* of ϕ.

Proposition 2.19. Let $\phi : G \to H$ be a homomorphism between groups G and H. The kernel $\mathrm{Ker}(\phi)$ is a normal subgroup of G.

[6]If N is normal, $(gn)(g'n') = (gg')(g'^{-1}ng')n' \in gg'N$.

Definition 2.3 (image)**.** Let $\phi : G \to H$ be a homomorphism between groups G and H. The set

$$\mathrm{Im}(\phi) := \{\phi(g) \mid g \in G\} \tag{27}$$

is called an *image* of ϕ.

Proposition 2.20. Let $\phi : G \to H$ be a homomorphism between groups G and H. The image $\mathrm{Im}(\phi)$ is a subgroup of H.

Theorem 2.21 (first isomorphism theorem)**.** *Let $\phi : G \to H$ be a homomorphism between groups G and H. Let N be the kernel of ϕ. There is an isomorphism $G/N \ni gN \mapsto \phi(g) \in \mathrm{Im}(\phi)$. That is, $G/N \cong \mathrm{Im}(\phi)$.*

We can construct a homomorphism between $\mathcal{A}_n$ and $\mathrm{O}(n)$ as

$$\varphi : \mathcal{A}_n \ni \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \mapsto \boldsymbol{A}\boldsymbol{W}\boldsymbol{A}^{-1} \in \mathrm{O}(n).$$

The kernel of φ is

$$\mathrm{Ker}(\varphi) = \mathcal{T}_n.$$

Thus, $\mathcal{A}_n/\mathcal{T}_n$ is isomorphic to $\mathrm{O}(n)$.

3 Group structure of space groups

3.1 Definition of space group

Let f be a crystal pattern. A space group of f is defined as the stabilizer on $\mathcal{E}_n$.

Definition 3.1 (space group)**.** The stabilizer of crystal pattern f on $\mathcal{E}_n$

$$\mathcal{G} := \mathrm{Stab}_{\mathcal{E}_n}(f) = \{g \in \mathcal{E}_n \mid gf = f\} \tag{28}$$

is called *space group* if $\mathcal{T}(\mathcal{G}) := \mathcal{T}_n \cap \mathcal{G}$ is isomorphic to a n-dimensional lattice. For the space group $\mathcal{G}$, $\mathcal{T}(\mathcal{G})$ is called *translation subgroup* of $\mathcal{G}$.

The above definition is for space groups in a broad sense. In a narrow sense, the space group of a stabilizer of a three-dimensional crystal pattern with a three-dimensional translational subgroup. The other symmetry groups for crystal patterns are summarized in Table 1.

Table 1: Symmetry groups of n-dimensional crystal patterns with r-dimensional translations.

n	r	Symmetry group	Table
2	1	Frieze group	Section 2.1 of ITE [11]
2	2	Plane group	Section 2.2 of ITA [1]
3	1	Rod group	Section 3.1 of ITE [11]
3	2	Layer group	Section 4.1 of ITE [11]
3	3	Space group	Section 2.3 of ITA [1]

3.2 Point group

Let $\mathcal{G}$ be a space group. The translation subgroup $\mathcal{T}(\mathcal{G})$ is normal subgroup of $\mathcal{G}$: For any $(\mathbf{W}, \mathbf{w}) \in \mathcal{G}$ and $(\mathbf{I}_n, \mathbf{t}) \in \mathcal{T}(\mathcal{G})$, one has

$$(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}_n, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w})^{-1} = (\boldsymbol{I}_n, \boldsymbol{W}\boldsymbol{t}) \in \mathcal{T}(\mathcal{G}). \tag{29}$$

Definition 3.2 (point group)**.** The set of the linear parts of a space group $\mathcal{G}$ is called *point group* of $\mathcal{G}$

$$\mathcal{P}(\mathcal{G}) := \{\mathbf{W} \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}. \tag{30}$$

The point group $\mathcal{P}(\mathcal{G})$ is isomorphic to the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$.

The homomorphism $\mathcal{G} \in (\boldsymbol{W}, \boldsymbol{w}) \mapsto \boldsymbol{W} \in \mathcal{P}(\mathcal{G})$ gives the isomorphism between $\mathcal{G}/\mathcal{T}(\mathcal{G})$ and $\mathcal{P}(\mathcal{G})$.

We fix some basis vectors $(\boldsymbol{a}_1, \dots, \boldsymbol{a}_n)$ of affine space, and act all mappings in point group $\mathcal{P}$ on the basis vectors. Since affine mappings in the point group $\mathcal{P}$ are isometry, it does not change the norm of vectors. Therefore, there are only finitely many acted vectors because the maximum norm of acted vectors is bound by $\max_{i=1,\dots,n} \mathbf{a}_i$.

Theorem 3.3. *The point group $\mathcal{P}$ of a space group $\mathcal{G}$ is finite.*

When we choose the lattice basis of $\mathcal{T}(\mathcal{G})$ as the basis vectors of the affine spaces, the translation subgroup $\mathcal{T}(\mathcal{G})$ is represented as $\{(\boldsymbol{I}_n, \boldsymbol{t}) \mid \boldsymbol{t} \in \mathbb{Z}^n\}$. And the action of point group $\mathcal{P}$ is described as integer matrices.

3.3 Symmorphic and non-symmorphic space groups

The translation subgroup of space group $\mathcal{G}$ can be chosen to be $\mathcal{T} = \mathbb{Z}^n$ by choosing primitive basis vectors. Also, the point group of $\mathcal{G}$ is a finite subgroup $\mathcal{P}$ of $\mathrm{GL}(n, \mathbb{Z})$. In general, a space group is not specified only with the translation subgroup $\mathcal{T}$ and point group $\mathcal{P}$. We need to determine a translation part $\boldsymbol{\tau}(\boldsymbol{W})$ of each linear part $\boldsymbol{W} \in \mathcal{P}$. We can construct $\mathcal{G}$ from $\mathcal{T}$, $\mathcal{P}$, and $\boldsymbol{\tau}$ as

$$\mathcal{G} = \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{\tau}(\boldsymbol{W}) + \boldsymbol{t} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \,\middle|\, \boldsymbol{W} \in \mathcal{P}, \boldsymbol{t} \in \mathbb{Z}^n \right\}. \tag{31}$$

Because the addition of lattice translation into $\boldsymbol{\tau}$ gives the same space group, it is sufficient to confine the range of $\boldsymbol{\tau}$ as $\boldsymbol{\tau} : \mathcal{P} \to [0, 1)^n$. Furthermore, the map $\boldsymbol{\tau}$ should satisfy a *cocycle condition*

$$\boldsymbol{\tau}(\boldsymbol{W}\boldsymbol{W}') \equiv \boldsymbol{\tau}(\boldsymbol{W}) + \boldsymbol{W}\boldsymbol{\tau}(\boldsymbol{W}') \pmod{\mathbb{Z}^n} \tag{32}$$

for all $\boldsymbol{W}, \boldsymbol{W}' \in \mathcal{P}$ so that a vector system consistent with the product of two symmetry operations:

$$\begin{pmatrix} \boldsymbol{W} & \boldsymbol{\tau}(\boldsymbol{W}) \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{W}' & \boldsymbol{\tau}(\boldsymbol{W}') \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}\boldsymbol{W}' & \boldsymbol{\tau}(\boldsymbol{W}) + \boldsymbol{W}\boldsymbol{\tau}(\boldsymbol{W}') \\ \boldsymbol{0}^\top & 1 \end{pmatrix}.$$

In particular, $\boldsymbol{\tau}(\boldsymbol{I}_n) \equiv \boldsymbol{0} \pmod{\mathbb{Z}^3}$.

Definition 3.4 (vector system [12])**.** Let $\mathcal{P}$ be a point group of a space group $\mathcal{G}$. The map $\boldsymbol{\tau} : \mathcal{P} \to \mathbb{R}^n$ is called a *vector system* if the map satisfies *cocycle condition* in Eq. (32).

In summary, a space group is fully constructed from its translation subgroup, point group, and vector system.

Note that the choice of the origin of the affine space transforms the translation part $\boldsymbol{\tau}$. When we change the origin from $\boldsymbol{O}$ to $\boldsymbol{O} + \boldsymbol{A}\boldsymbol{p}$, a symmetry operation $(\boldsymbol{W}, \boldsymbol{\tau}(\boldsymbol{W}))$

are transformed to

$$\begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{p} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}^{-1} \begin{pmatrix} \boldsymbol{W} & \boldsymbol{\tau}(\boldsymbol{W}) \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{p} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W} & \boldsymbol{\tau}(\boldsymbol{W}) + (\boldsymbol{W} - \boldsymbol{I}_n)\boldsymbol{p} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}$$

from Eq. (13). Thus, for any $\boldsymbol{p} \in \mathbb{R}^n$, a vector system

$$\boldsymbol{\tau}_{\boldsymbol{p}}(\boldsymbol{W}) \coloneqq \boldsymbol{\tau}(\boldsymbol{W}) + (\boldsymbol{W} - \boldsymbol{I}_n)\boldsymbol{p} \quad (\boldsymbol{W} \in \mathcal{P}) \tag{33}$$

and $\boldsymbol{\tau}$ give the same space group.

Definition 3.5 (symmorphic and non-symmorphic)**.** Let $\boldsymbol{\tau}$ be a vector system of a space group $\mathcal{G}$. If there exists an origin shift $\boldsymbol{p} \in \mathbb{R}^n$ such that $\boldsymbol{\tau}_{\boldsymbol{p}} \equiv \boldsymbol{0}$, $\mathcal{G}$ is called a *symmorphic* space group. Otherwise, $\mathcal{G}$ is called a *non-symmorphic* space group.

3.4 Working examples from plane groups

Let us derive plane groups $p2mm$, $p2mg$ and $p2gg$ from a translation group $\mathbb{Z}^2$ and a point group

$$\mathcal{P}_{\mathrm{2mm}} = \left\{ \boldsymbol{W}_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \boldsymbol{W}_1 = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \boldsymbol{W}_2 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \boldsymbol{W}_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right\}.$$

This example is adopted from Section 4.2 of Ref. [3].

Let $\boldsymbol{\tau}_i = \boldsymbol{\tau}(\boldsymbol{W}_i)$ for $i = 1, \ldots, 4$. It is sufficient to consider $\boldsymbol{\tau}_2 = \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$ and $\boldsymbol{\tau}_3 = \begin{pmatrix} a_3 \\ b_3 \end{pmatrix}$ because the remains are obtained from the cocycle condition,

$$\boldsymbol{\tau}_1 = \boldsymbol{\tau}(\boldsymbol{W}_2\boldsymbol{W}_3) = \boldsymbol{\tau}_2 + \boldsymbol{W}_2\boldsymbol{\tau}_3 = \begin{pmatrix} a_2 - a_3 \\ b_2 + b_3 \end{pmatrix}.$$

The relation $\boldsymbol{W}_2^2 = \boldsymbol{W}_0$ gives

$$\begin{aligned} \boldsymbol{\tau}_0 = \boldsymbol{\tau}(\boldsymbol{W}_2^2) = \boldsymbol{\tau}_2 + \boldsymbol{W}_2\boldsymbol{\tau}_2 = \begin{pmatrix} 0 \\ 2b_2 \end{pmatrix} \\ \therefore 2b_2 \equiv 0 \pmod{\mathbb{Z}}. \end{aligned}$$

The relation $\boldsymbol{W}_3^2 = \boldsymbol{W}_0$ gives

$$\begin{aligned} \boldsymbol{\tau}_0 = \boldsymbol{\tau}_3 + \boldsymbol{W}_3\boldsymbol{\tau}_3 = \begin{pmatrix} 2a_3 \\ 0 \end{pmatrix} \\ \therefore 2a_3 \equiv 0 \pmod{\mathbb{Z}}. \end{aligned}$$

The relation $(\boldsymbol{W}_2\boldsymbol{W}_3)^2 = \boldsymbol{W}_1^2 = \boldsymbol{W}_0$ gives no restriction,

$$\boldsymbol{\tau}_0 = \boldsymbol{\tau}_1 + \boldsymbol{W}_1\boldsymbol{\tau}_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

The trivial vector system $\boldsymbol{\tau}^0_{\boldsymbol{p},i} = (\boldsymbol{W}_i - \boldsymbol{I})\boldsymbol{p} \quad (i = 1, \ldots, 4)$ for origin shift $\boldsymbol{p} = \begin{pmatrix} p \\ q \end{pmatrix}$ is computed as

$$\boldsymbol{\tau}^0_{\boldsymbol{p},0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\tau}^0_{\boldsymbol{p},1} = \begin{pmatrix} -2p \\ -2q \end{pmatrix}, \boldsymbol{\tau}^0_{\boldsymbol{p},2} = \begin{pmatrix} -2p \\ 0 \end{pmatrix}, \boldsymbol{\tau}^0_{\boldsymbol{p},3} = \begin{pmatrix} 0 \\ -2q \end{pmatrix}.$$

. Thus, we can choose $p = -\frac{a_2}{2}, q = -\frac{b_3}{2}$ so that $a_2 = b_3 = 0$. We derived the following vector systems

- $\boldsymbol{\tau}_2 = \boldsymbol{\tau}_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: *p*2*mm*
- $\boldsymbol{\tau}_2 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \boldsymbol{\tau}_3 = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: *p*2*mg* (reflection along a axis and glide along b axis)
- $\boldsymbol{\tau}_2 = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \boldsymbol{\tau}_3 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$: *p*2*mg* (reflection along b axis and glide along a axis)
- $\boldsymbol{\tau}_2 = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}, \boldsymbol{\tau}_3 = \begin{pmatrix} 0 \\ \frac{1}{2} \end{pmatrix}$: *p*2*gg*.

4 Classification of space groups

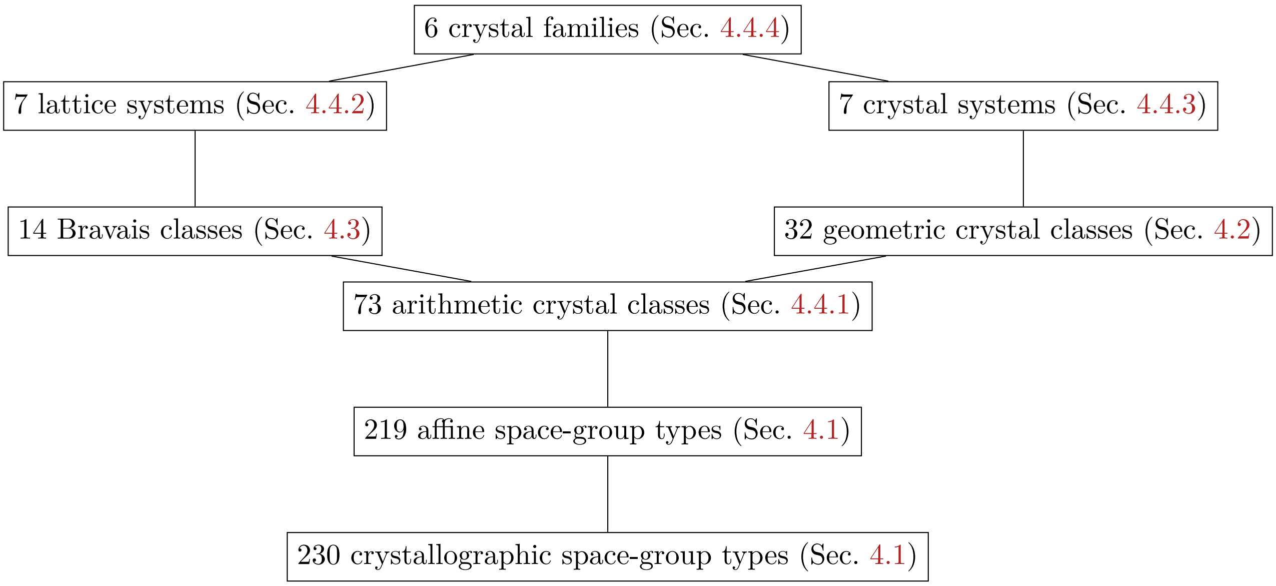

Figure 3: Classification of space groups

We classify space groups in three dimensions (see Fig. 3 for the hierarchy of the classifications).

4.1 Affine space-group type and space-group type

It is natural to identify two space groups that are transformed into another by changing coordinate systems.

Definition 4.1 (affine space-group type)**.** Two space groups $\mathcal{G}, \mathcal{G}'$ belong to the same *affine space-group type* if they are conjugate by some affine mapping $(\boldsymbol{P}, \boldsymbol{p}) \in \mathcal{A}_3$ such that

$$(\boldsymbol{P}, \boldsymbol{p})^{-1} \mathcal{G} (\boldsymbol{P}, \boldsymbol{p}) = \mathcal{G}'. \tag{34}$$

These space groups are also called *affinely equivalent*.

It is nontrivial fact that affine equivalence completely identifies the isomorphism of space groups.

Theorem 4.2 (Bieberbach)**.** *Two space groups are isomorphic if and only if they belong to the same affine type.*

In crystallography, a tighter classification of space groups is often used. That is, orientation-preserving affine mapping is only considered in transformations of coordinates systems[7].

Definition 4.3 (space-group type)**.** Two space groups $\mathcal{G}, \mathcal{G}'$ belong to the same *(crystallographic) space-group type* if they are conjugate by some orientation-preserving affine mapping $(\boldsymbol{P}, \boldsymbol{p}) \in \mathcal{A}_3^+$ such that $(\boldsymbol{P}, \boldsymbol{p})^{-1}\mathcal{G}(\boldsymbol{P}, \boldsymbol{p}) = \mathcal{G}'$, where orientation-preserving affine mapping is an affine mapping whose linear part is positive,

$$\mathcal{A}_n^+ := \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \middle| \boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \det \boldsymbol{W} > 0, \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{35}$$

A pair of affine space-groups types that belong to the different crystallographic space-group types are called *enantiomorphic pair*. For example, there are 11 enantiomorphic pairs in three dimensions as Table. 2.

Table 2: Enantiomorphic pairs in space groups

$P4_1$ (76)	$P4_3$ (78)
$P4_122$ (91)	$P4_322$ (95)
$P4_12_12$ (92)	$P4_32_12$ (96)
$P3_1$ (144)	$P3_2$ (145)
$P3_112$ (151)	$P3212$ (153)
$P3_121$ (152)	$P3_221$ (154)
$P6_1$ (169)	$P6_5$ (173)
$P6_2$ (170)	$P6_4$ (172)
$P6_122$ (178)	$P6_522$ (179)
$P6_222$ (180)	$P6_422$ (181)
$P4_332$ (212)	$P4_132$ (213)

4.2 Classification based on point group

We consider classification based on a point group of a space group.

[7]Some people indicate “space groups” as space-group types in their terminology. I think the clear distinction between space groups and space-group types makes our lives easier.

Definition 4.4 (geometric crystal class)**.** Two subgroups of $\mathrm{GL}(3,\mathbb{Z})$, $\mathcal{P}$ and $\mathcal{P}'$, belong to the same *geometric crystal class* if they are conjugate by some invertible matrix $\boldsymbol{P} \in \mathrm{GL}(3,\mathbb{R})$ such that

$$\boldsymbol{P}^{-1}\mathcal{P}\boldsymbol{P} = \mathcal{P}'. \tag{36}$$

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, respectively, belong to the same *geometric crystal class* if $\mathcal{P}$ and $\mathcal{P}'$ belong to the same geometric crystal class.

There are 32 geometric crystal classes for space groups shown in Table 7.

Two space groups belong to the same *Laue class* if point groups obtained by their point group with inversions belong to the same geometric crystal class (Table 3).

Table 3: Laue classes in space groups

Laue class	Geometric crystal class
$\overline{1}$	1, $\overline{1}$
$2/m$	2, m, $2/m$
mmm	222, $2mm$, mmm
$\overline{3}$	3, $\overline{3}$
$\overline{3}m$	32, $3m$, $\overline{3}m$
$4/m$	4, $\overline{4}$, $4/m$
$4/mmm$	422, $\overline{4}2m$, $4mm$, $4/mmm$
$6/m$	6, $\overline{6}$, $6/m$
$6/mmm$	622, $\overline{6}2m$, $6mm$, $6/mmm$
$m\overline{3}$	23, $m\overline{3}$
$m\overline{3}m$	432, $\overline{4}32$, $m\overline{3}m$

Example: point groups of $P\overline{4}2m$ and $P\overline{4}m2$ The point group of space-group type $P\overline{4}2m$ is generated from fourfold rotoinversion along the c axis and twofold rotation along the a axis,

$$\overline{4}^{+}_{001} : \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, 2_{100} : \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

On the other hand, the point group of space-group type $P\overline{4}m2$ is generated from fourfold rotoinversion along the c axis and twofold rotation along the [110] axis,

$$\overline{4}^{+}_{001} : \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, 2_{110} : \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

These two point groups $\overline{4}2m$ and $\overline{4}m2$ are conjugated by $\frac{\pi}{4}$ rotation along the c axis. Thus, they belong to the same geometric crystal class $\overline{4}2m$. However, $P\overline{4}2m$ and $P\overline{4}m2$ belong to different space-group types because the $\frac{\pi}{4}$ rotation cannot act on the lattice.

Example: *pm* and *cm* The point group of both plane-group types pm and cm is generated from

$$m : \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{37}$$

Thus, pm and cm belong to the same geometric crystal class m.

4.3 Classification based on lattice

4.3.1 Bravais group and Bravais type of lattice

We consider classification based on a translation lattice of a space group.

Definition 4.5 (translation lattice)**.** A *translation lattice* L of a space group $\mathcal{G}$ is a set of translation parts of translation subgroup of $\mathcal{G}$,

$$L = \{ \boldsymbol{A}\boldsymbol{t} \mid (\boldsymbol{I}_3, \boldsymbol{t}) \in \mathcal{G} \}. \tag{38}$$

Definition 4.6 (Bravais group)**.** Let $\boldsymbol{G}$ be a metric tensor of a translation lattice L with primitive basis vectors. A set of isometry mapping that preserves L is called the *Bravais group* of L,

$$\mathcal{B}(L) := \left\{ \boldsymbol{W} \in \mathrm{GL}(3, \mathbb{Z}) \,\middle|\, \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G} \right\}. \tag{39}$$

Note that the Bravais group may change as a set by transforming primitive basis.

Definition 4.7 (Bravais type of lattice)**.** Two lattices L and L' belong to the same *Bravais type of lattice* if their Bravais groups are conjugate by some unimodular matrix $\boldsymbol{P} \in \mathrm{SL}(3, \mathbb{Z})$ such that

$$\boldsymbol{P}^{-1} \mathcal{B}(L) \boldsymbol{P} = \mathcal{B}(L'). \tag{40}$$

This definition of Bravais types of lattices is independent of choices for primitive basis.

Example: Bravais types of lattices of translation lattices of *pm* and *cm* We consider a translation lattice of pm. We assume cell parameters a and b have no relationship to each other. The metric tensor for one of the choices of primitive basis vectors is

$$\boldsymbol{G}_{pm} = \begin{pmatrix} a^2 & 0 \\ 0 & b^2 \end{pmatrix}.$$

The Bravais group of L_{pm} is

$$\mathcal{B}(L_{pm}) = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \right\}. \tag{41}$$

Next, we consider a translation lattice of cm, L_{cm}. We transform a conventional cell with cell parameter $\gamma = 90°$ to a primitive cell by $(\boldsymbol{a}_p, \boldsymbol{b}_p) = (\boldsymbol{a}, \boldsymbol{b})\boldsymbol{P}$ with

$$\boldsymbol{P} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

The metric tensor with the primitive basis vectors is

$$\boldsymbol{G}_{cm} = \begin{pmatrix} \frac{a^2+b^2}{2} & \frac{a^2-b^2}{2} \\ \frac{a^2-b^2}{2} & \frac{a^2+b^2}{2} \end{pmatrix}.$$

The Bravais group of L_{cm} with the primitive basis vectors is

$$\mathcal{B}(L_{cm}) = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \right\}. \tag{42}$$

The two Bravais groups $\mathcal{B}(L_{pm})$ and $\mathcal{B}(L_{cm})$ are conjugate by $\frac{\pi}{4}$ rotation, which does not belong to $\mathrm{SL}(3, \mathbb{Z})$. Thus, L_{pm} and L_{cm} belong to the different Bravais types of lattices (*op* and *oc*). The Bravais groups for two-dimensional lattices are given in Table 4.

Table 4: The Bravais groups of two-dimensional lattices (Table 1.3.3.1 of Ref. [1])

Lattice	Metric tensor	Bravais group
oblique	$\begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix}$	2
rectangular	$\begin{pmatrix} g_{11} & 0 \\ 0 & g_{22} \end{pmatrix}$	$2mm$
square	$\begin{pmatrix} g_{11} & 0 \\ 0 & g_{11} \end{pmatrix}$	$4mm$
hexagonal	$\begin{pmatrix} g_{11} & -\frac{1}{2}g_{11} \\ -\frac{1}{2}g_{11} & g_{11} \end{pmatrix}$	$6mm$

4.3.2 Bravais type of lattice and Bravais class

Definition 4.8 (Bravais manifold)**.** Let K be a subgroup of $\mathrm{GL}(3,\mathbb{Z})$. A *space of metric tensors (Bravais manifold) of* K is the space of all metric tensors invariant with K,

$$\boldsymbol{M}(K) := \left\{ \boldsymbol{G} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \,\middle|\, \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G} \quad (\forall \boldsymbol{W} \in K) \right\} \tag{43}$$

Let L and $\mathcal{P}$ be a translation lattice and a point group of a space group $\mathcal{G}$, respectively. When the dimension of $\boldsymbol{M}(\mathcal{B}(L))$ is smaller than that of $\boldsymbol{M}(\mathcal{P})$, the translation lattice L is called to have *spaciealized metric*.

Definition 4.9 (Bravais class)**.** Let L be some lattice with a metric tensor $\boldsymbol{G}$. A space group $\mathcal{G}$ with a point group $\mathcal{P}$ belongs to a *Bravais class* corresponding to the Bravais type of L if $\boldsymbol{M}(\mathcal{P})$ and $\boldsymbol{M}(\mathcal{B}(L))$ are conjugate by some unimodular matrix $\boldsymbol{P} \in \mathrm{SL}(3,\mathbb{Z})$ such that

$$\boldsymbol{P}^{-1}\boldsymbol{M}(\mathcal{P})\boldsymbol{P} = \boldsymbol{M}(\mathcal{B}(L)). \tag{44}$$

Note that the definition of Bravais classes is independent of whether a translation lattice is a specialized metric or not.

Definition 4.10 (holohedry)**.** A subgroup $\mathcal{P}$ of $\mathrm{GL}(3,\mathbb{Z})$ is called *holohedry* if there is a lattice L whose Bravais group belongs to the same geometric crystal class of $\mathcal{P}$.

The seven holohedries for the three-dimensional lattices are shown in Table. 6.

Example: Bravais manifolds and Bravais classes of *pm* The Bravais manifold of the Bravais group in Eq. (41) is

$$\boldsymbol{M}(\mathcal{B}(L_{pm})) = \left\{ \begin{pmatrix} g_{11} & 0 \\ 0 & g_{22} \end{pmatrix} \,\middle|\, g_{11}, g_{22} \in \mathbb{R} \right\}.$$

If the metric tensor satisfies $g_{11} = g_{22}$ $(a = b)$, the corresponding Bravais group is $4mm$. The Bravais manifold of $4mm$ has only one free parameter. Thus, such a lattice has a specialized metric.

The Bravais manifold of the point group of pm is

$$\boldsymbol{M}(\mathcal{P}_{pm}) = \left\{ \begin{pmatrix} g_{11} & 0 \\ 0 & g_{22} \end{pmatrix} \,\middle|\, g_{11}, g_{22} \in \mathbb{R} \right\}.$$

Therefore, pm belongs to the Bravais group *op* whether its translation lattice has a specialized metric or not.

Example: Bravais manifolds and Bravais classes of cm The Bravais manifold of the Bravais group in Eq. (42) is

$$\boldsymbol{M}(\mathcal{B}(L_{cm})) = \left\{ \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{11} \end{pmatrix} \middle| \, g_{11}, g_{12} \in \mathbb{R} \right\}.$$

If $g_{12} = 0 \, (a = b)$, the corresponding Bravais group is $4mm$. If $g_{12} = -\frac{1}{2} g_{11} \, (b = \sqrt{3}a)$, the corresponding Bravais group is $6mm$.

The Bravais manifold of the point group of cm is

$$\boldsymbol{M}(\mathcal{P}_{pm}) = \left\{ \begin{pmatrix} g_{11} & 0 \\ 0 & g_{22} \end{pmatrix} \middle| \, g_{11}, g_{22} \in \mathbb{R} \right\}.$$

Therefore, cm belongs to the Bravais group oc whether its translation lattice has a specialized metric or not.

4.4 Other classifications

4.4.1 Arithmetic crystal class

Definition 4.11 (arithmetic crystal class)**.** Two subgroups of $\mathrm{GL}(3, \mathbb{Z})$, $\mathcal{P}$ and $\mathcal{P}'$, belong to the same *arithmetic crystal class* if they are conjugate by some unimodular matrix $\boldsymbol{P} \in \mathrm{SL}(3, \mathbb{Z})$ such that

$$\boldsymbol{P}^{-1} \mathcal{P} \boldsymbol{P} = \mathcal{P}'. \tag{45}$$

Two space groups $\mathcal{G}$ and $\mathcal{G}'$ with point groups $\mathcal{P}$ and $\mathcal{P}'$, both written with primitive basis vectors, belong to the same *arithmetic crystal class* if $\mathcal{P}$ and $\mathcal{P}'$ belong to the same arithmetic crystal class.

The arithmetic crystal class forgets vector systems of space groups in Sec. 3.3. Therefore, the arithmetic crystal classes have a one-to-one correspondence with symmorphic space-group types. There are 73 arithmetic crystal classes for space groups.

Definition 4.12 (Bravais arithmetic crystal class)**.** The arithmetic crystal class of a space group $\mathcal{G}$ is called a *Bravais arithmetic crystal class* if the point group of $\mathcal{G}$ is the Bravais group of the translation lattice L of $\mathcal{G}$,

$$\mathcal{P} = \mathcal{B}(L). \tag{46}$$

The definition of Bravais arithmetic crystal classes is compatible with that of Bravais types of lattices (see Table 5).

Table 5: The correspondence of Bravais arithmetic crystal classes and Bravais types of lattices in three dimensions.

Bravais type of lattice	Bravais arithmetic crystal class
aP	$\overline{1}P$
mP	$2/mP$
mC	$2/mC$
oP	$mmmP$
oS	$mmmC$
oF	$mmmF$
oI	$mmmI$
tP	$4/mmmP$
tI	$4/mmmI$
hR	$\overline{3}mR$
hP	$6/mmmP$
cP	$m\overline{3}mP$
cF	$m\overline{3}mF$
cI	$m\overline{3}mI$

4.4.2 Lattice system

Definition 4.13 (lattice system)**.** Two lattices L and L' belong to the same *lattice system* if their Bravais groups belong to the same geometric crystal class, that is, some invertible matrix $\boldsymbol{P} \in \mathrm{GL}(3, \mathbb{R})$ exists such that

$$\boldsymbol{P}^{-1}\mathcal{B}(L)\boldsymbol{P} = \mathcal{B}(L'). \tag{47}$$

Two Bravais classes belong to the same *lattice system* if the corresponding Bravais arithmetic crystal classes belong to the same holohedry. There are seven lattice systems for three-dimensional space groups as shown in Table 6.

Table 6: Lattice systems in the three-dimensional space

Lattice system	Holohedry	Bravias types of lattices
Triclinic	$\overline{1}$	aP
Monoclinic	$2/m$	mP, mS
Orthorhombic	mmm	oP, oS, oF, oI
Tetragonal	$4/mmm$	tP, tI
Rhombohedral	$\overline{3}m$	hR
Hexagonal	$6/mmm$	hP
Cubic	$m\overline{3}m$	cP, cF, cI

4.4.3 Crystal system

Definition 4.14 (crytal system)**.** Two space groups with point groups $\mathcal{P}$ and $\mathcal{P}'$ belong to the same *crystal system* if and only if the sets of Bravais type of lattices on which these point groups act coincide.

There are seven crystal systems for three-dimensional space groups as shown in Table 7.

Table 7: Crystal systems in space groups

Crystal system	Geometric crystal classes
Triclinic	$1, \overline{1}$
Monoclinic	$2/m, m, 2$
Orthorhombic	$mmm, mm2, 222$
Tetragonal	$4/mmm, \overline{4}2m, 4mm, 422, 4/m, \overline{4}, 4$
Hexagonal	$6/mmm, \overline{6}2m, 6mm, 622, 6/m, \overline{6}, 6$
Trigonal	$\overline{3}m, 3m, 32, \overline{3}, 3$
Cubic	$m\overline{3}m, \overline{4}3m, 432, m\overline{3}, 23$

4.4.4 Crystal family

Definition 4.15 (crystal family)**.** The *crystal family* of space group $\mathcal{G}$ is the union of all geometric crystal classes that contain some space group $\mathcal{G}'$ that has the same Bravais type of lattices as $\mathcal{G}$.

The hexagonal and trigonal crystal systems belong to the same crystal family, called the hexagonal crystal family, because a translation lattice of a trigonal space group with a specialized metric can have the Bravais group, $6/mmm$. There are six crystal families for the three-dimensional space groups: triclinic, monoclinic, orthorhombic, tetragonal, hexagonal, and cubic. Also, the hexagonal crystal family is shown in Table 8.

Table 8: Arithmetic crystal classes belonging to the hexagonal crystal family.

Crystal system \Lattice system	Hexagonal	Rhombohedral
Hexagonal	$6/mmmP$, $\overline{6}m2P$, $6mmP$, $622P$, $6/mP$, $\overline{6}P$, $6P$	
Trigonal	$\overline{3}mP$, $3mP$, $32P$, $\overline{3}P$, $3P$	$\overline{3}mR$, $3mR$, $32R$, $\overline{3}R$, $3R$

5 Conventions for space groups

5.1 Conventional cell

5.2 Helmann–Mauguin symbol

TODO: Section 1.4.2 of ITA

Convention for Hermann-Mauguin symbols is shown in Table 9.

Table 9: lattice symmetry directions in three-dimensional space (ITA Table 2.1.3.1)

Lattice system	Primary	Secondary	Tertiary
triclinic	None		
monoclinic (unique axis b)	[010]		
orthorhombic	[100]	[010]	[001]
tetragonal	[001]	$\langle 100\rangle = [100][010]$	$\langle 1\bar{1}0\rangle = [110][1\bar{1}0]$
rhombohedral(hexagonal axes)	[001]	$\langle 100\rangle = [100][010][\bar{1}\bar{1}0]$	
rhombohedral(rhombohedral axes)	[111]	$\langle 1\bar{1}0\rangle = [1\bar{1}0][01\bar{1}][\bar{1}01]$	
hexagonal	[001]	$\langle 100\rangle = [100][010][\bar{1}\bar{1}0]$	$\langle 1\bar{1}0\rangle = [1\bar{1}0][120][\bar{2}\bar{1}0]$
cubic	$\langle 001\rangle = [100][010][001]$	$\langle 111\rangle = [111][1\bar{1}\bar{1}][\bar{1}1\bar{1}][\bar{1}\bar{1}1]$	$\langle 110\rangle = [1\bar{1}0][110][01\bar{1}][011][\bar{1}01][101]$

TODO: How to read H-M symbols

5.3 Alternative descriptions of space groups in ITA

5.3.1 Monoclinic system(ITA-2.1.3.15)

TODO: Fix unique axes

Axis settings for monoclinic systems are shown in Table 10. Cell choices for monoclinic systems are shown in Table 11 and Fig. 4.

Table 10: settings of monoclinic system

unique axis setting	$\mathbf{b}$ $\mathbf{a}\underline{\mathbf{b}}\mathbf{c}$	$-\mathbf{b}$ $\mathbf{c}\underline{\bar{\mathbf{b}}}\mathbf{a}$	$\mathbf{c}$ $\mathbf{a}\mathbf{b}\underline{\mathbf{c}}$	$-\mathbf{c}$ $\mathbf{b}\mathbf{a}\underline{\bar{\mathbf{c}}}$	$\mathbf{a}$ $\underline{\mathbf{a}}\mathbf{b}\mathbf{c}$	$-\mathbf{a}$ $\underline{\bar{\mathbf{a}}}\mathbf{b}\mathbf{c}$
transformation to $\mathbf{a}\underline{\mathbf{b}}\mathbf{c}$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&0&1\\0&-1&0\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&1\\0&-1&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&-1&0\\1&0&0\\0&0&1\end{pmatrix}$
Cell choice 1	$C \to C$	$A \to C$	$A \to C$	$B \to C$	$B \to C$	$C \to C$
Cell choice 2	$A \to A$	$C \to A$	$B \to A$	$A \to A$	$C \to A$	$B \to A$
Cell choice 3	$I \to I$	$I \to I$	$I \to I$	$I \to I$	$I \to I$	$I \to I$

Table 11: transformation of cell choices in monoclinic system

choice	$b1$	$b2$	$b3$
transformation to $b1$	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}-1&0&1\\0&1&0\\-1&0&0\end{pmatrix}$	$\begin{pmatrix}0&0&-1\\0&1&0\\1&0&-1\end{pmatrix}$
centering	$C \to C$	$A \to C$	$I \to C$

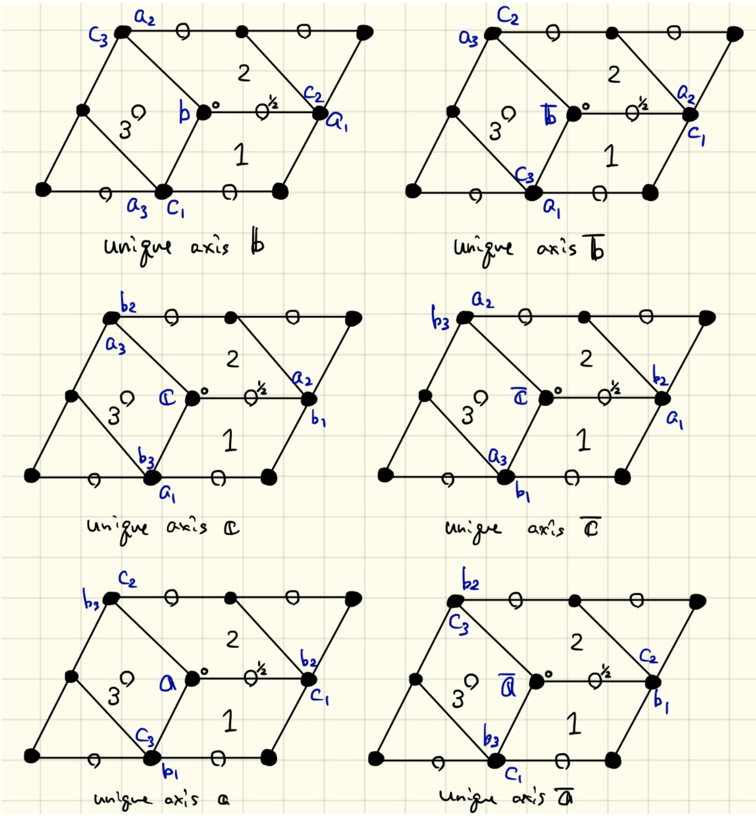

Figure 4: choices of monoclinic system

5.3.2 Orthorhombic system

Axis settings for orthorhombic systems are shown in Table 12.

5.3.3 Standard ITA setting

The standard ITA setting is one of the conventional descriptions for each space-group type used in the *International Tables for Crystallography Vol. A* [1]: unique axis b setting, cell choice 1 for monoclinic groups, hexagonal axes for rhombohedral groups, and origin choice 2 for centrosymmetric groups.

5.4 Hall symbol

Table 12: settings of orthorhombic system

settings	$\mathbf{abc}$	$\mathbf{ba\bar{c}}$	$\mathbf{cab}$	$\mathbf{\bar{c}ba}$	$\mathbf{bca}$	$\mathbf{a\bar{c}b}$
transformation to **abc**	$\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}$	$\begin{pmatrix}0&1&0\\1&0&0\\0&0&-1\end{pmatrix}$	$\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix}$	$\begin{pmatrix}0&0&-1\\0&1&0\\1&0&0\end{pmatrix}$	$\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix}$	$\begin{pmatrix}1&0&0\\0&0&-1\\0&1&0\end{pmatrix}$
centering	$A \to A$ $B \to B$ $C \to C$	$A \to B$ $B \to A$ $C \to C$	$A \to C$ $B \to A$ $C \to B$	$A \to C$ $B \to B$ $C \to A$	$A \to B$ $B \to C$ $C \to A$	$A \to A$ $B \to C$ $C \to B$

6 Magnetic space group

6.1 Definition

We consider a *time-reversal operation* $1'$ and call an index-two group generated from $1'$ as a *time-reversal group* $\{1, 1'\}\,(\cong \mathbb{Z}_2)$, where 1 represents an identity operation. Let $\mathcal{M}$ be a subgroup of a direct product of E(3) and $\{1, 1'\}$. An element $(\boldsymbol{W}, \boldsymbol{w})\theta$ of $\mathcal{M}$ is called a *magnetic symmetry operation*, where $\theta \in \{1, 1'\}$ is a *time-reversal part* of the magnetic symmetry operation. A translation subgroup of $\mathcal{M}$ is defined similarly as

$$\mathcal{T}(\mathcal{M}) \coloneqq \{(\boldsymbol{E}, \boldsymbol{t}) \mid \exists\theta \in \{1, 1'\}, (\boldsymbol{E}, \boldsymbol{t})\theta \in \mathcal{M}\}\,. \tag{48}$$

The subgroup $\mathcal{M}$ is called a *magnetic space group* (MSG) when its translation subgroup is generated from three independent translations. We write a *magnetic point group* of $\mathcal{M}$ as

$$\mathcal{P}(\mathcal{M}) \coloneqq \left\{\boldsymbol{W}\theta \,\middle|\, \exists\boldsymbol{w} \in \mathbb{R}^3, (\boldsymbol{W}, \boldsymbol{w})\theta \in \mathcal{M}\right\}. \tag{49}$$

We consider two derived space groups from $\mathcal{M}$. A *family space group* (FSG) of $\mathcal{M}$ is a space group obtained by ignoring time-reversal parts in magnetic symmetry operations:

$$\mathcal{F}(\mathcal{M}) \coloneqq \{(\boldsymbol{W}, \boldsymbol{w}) \mid \exists\theta \in \{1, 1'\}, (\boldsymbol{W}, \boldsymbol{w})\theta \in \mathcal{M}\}\,. \tag{50}$$

A *maximal space subgroup* (XSG) of $\mathcal{M}$ is a space group obtained by removing antisymmetry operations:

$$\mathcal{D}(\mathcal{M}) \coloneqq \{(\boldsymbol{W}, \boldsymbol{w}) \mid (\boldsymbol{W}, \boldsymbol{w})1 \in \mathcal{M}\}\,. \tag{51}$$

6.2 Type of magnetic space group

The MSGs are classified into the following four types:

- (Type I) $\mathcal{M} = \mathcal{F}(\mathcal{M})1 = \mathcal{D}(\mathcal{M})1$: The MSG $\mathcal{M}$ does not have antisymmetry operations.
- (Type II) $\mathcal{M} = \mathcal{F}(\mathcal{M})1 \sqcup \mathcal{F}(\mathcal{M})1', \mathcal{F}(\mathcal{M}) = \mathcal{D}(\mathcal{M})$: The MSG $\mathcal{M}$ has antisymmetry operations and corresponding ordinary symmetry operations.
- (Type III) $\mathcal{M} = \mathcal{D}(\mathcal{M})1 \sqcup (\mathcal{F}(\mathcal{M}) \backslash \mathcal{D}(\mathcal{M}))1'$ and $\mathcal{D}(\mathcal{M})$ is an index-two *translationengleiche* subgroup of $\mathcal{F}(\mathcal{M})$. Thus, translation subgroups of $\mathcal{F}(\mathcal{M})$ and $\mathcal{D}(\mathcal{M})$ are identical.
- (Type IV) $\mathcal{M} = \mathcal{D}(\mathcal{M})1 \sqcup (\mathcal{F}(\mathcal{M}) \backslash \mathcal{D}(\mathcal{M}))1'$ and $\mathcal{D}(\mathcal{M})$ is an index-two *klassengleiche* subgroup of $\mathcal{F}(\mathcal{M})$. Thus, point groups of $\mathcal{F}(\mathcal{M})$ and $\mathcal{D}(\mathcal{M})$ are identical.

For a type-III MSG example, consider $\mathcal{M}_{\text{rutile}} = \overline{P}4'_n2'_n$ (BNS number 136.498) in magnetic Hall symbols. The FSG and XSG of $\mathcal{M}_{\text{rutile}}$ are $\overline{P}4_n2_n$ (No. 136) and $\overline{P}22_n$ (No. 58) in Hall symbols, respectively.

For a type-IV MSG example, consider $\mathcal{M}_{\text{bcc}} = \overline{P}4231'_n$ (BNS number 221.97) in magnetic Hall symbols. The FSG and XSG of $\mathcal{M}_{\text{bcc}}$ are $\overline{I}423$ (No. 229) and $\overline{P}423$ (No. 221) in Hall symbols, respectively.

6.3 BNS and OG symbols

The BNS symbol represents each magnetic space-group type [13]. We refer to a setting of the BNS symbol as a BNS setting: For types-I, -II, and -III MSGs, it uses the same setting as the standard ITA setting of the FSG. For type-IV MSG, it uses that of the XSG.

TODO: Add table to compare BNS and OG symbols

6.4 Magnetic Hall symbol

7 Site symmetry group and normalizer

7.1 Euclidean normalizer and affine normalizer

7.2 Wyckoff set, equivalent descriptions of crystal structure

7.3 Normalizer action on vector system

Section 4.3 of Ref. [3]

7.4 Derivation of Euclidean normalizer

If $(\boldsymbol{P}, \boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$, for all $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$, there exists a symmetry operation $(\boldsymbol{W}', \boldsymbol{w}') in \mathcal{G}$ such that

$$\det \boldsymbol{P} \neq 0 \tag{52}$$

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{W}', \boldsymbol{w}'), \tag{53}$$

where

$$\boldsymbol{W}' = \boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{-1} \tag{54}$$

$$\boldsymbol{w}' = \boldsymbol{p} + \boldsymbol{P}\boldsymbol{w} - \boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{-1}\boldsymbol{p}. \tag{55}$$

7.4.1 Basis vectors of Euclidean normalizer

If $(\boldsymbol{E}|\boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$, for all $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{S}$, there exists a symmetry operation $(\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{S}$ such that

$$\boldsymbol{W}' = \boldsymbol{W} \tag{56}$$

$$\boldsymbol{w}' = \boldsymbol{p} + \boldsymbol{w} - \boldsymbol{W}\boldsymbol{p}. \tag{57}$$

When we take a primitive basis, the translation lattice is identified as $\mathbb{Z}^n$. If $(\boldsymbol{W}, \boldsymbol{w}), (\boldsymbol{W}, \boldsymbol{w}') \in \mathcal{S}$,

$$(\boldsymbol{W}, \boldsymbol{w}')^{-1}(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{E}, \boldsymbol{w} - \boldsymbol{w}') \in \mathcal{S}. \tag{58}$$

Thus, $\mathbf{w} - \mathbf{w}' \in \mathbb{Z}^n$.

In summary, the condition that $(\boldsymbol{E}, \boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$ is equivalent to

$$(\boldsymbol{E} - \boldsymbol{W})\boldsymbol{p} = \boldsymbol{0} (\mathrm{mod}\, \mathbb{Z}^n) \tag{59}$$

for all $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}$.

Conversely, a set of operations $(\boldsymbol{E}, \boldsymbol{p})$ satisfying Eq. (59) is a subgroup of $\mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$.

The linear integer system of Eq. (59) can be solved by its Hermite or Smith normal form (see Sec. 8.2.5).

Because the above discussion is independent of whether an operation is an isometry or not, basis vectors of the Euclidean normalizer and affine normalizer can coincide.

7.4.2 Linear part of Euclidean normalizer

If $(\boldsymbol{P}, \boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$, for all $(\boldsymbol{E}, \boldsymbol{w}) \in \mathcal{S}$, $(\boldsymbol{P}, \boldsymbol{p})$ satisfies the following condition at least

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{E}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{E}, \boldsymbol{P}\boldsymbol{w}) \in \mathcal{G}. \tag{60}$$

Therefore, $\boldsymbol{P} \in \mathrm{GL}_n(\mathbf{Z})$.

Similarly, considering $(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{P}^{-1}, -\boldsymbol{P}^{-1}\boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{S})$, we obtain $\boldsymbol{A}^{-1} \in \mathrm{GL}_n(\mathbf{Z})$. Thus, $\boldsymbol{P}$ is a unimodular (integer) matrix.

Moreover, $\boldsymbol{P}$ should belong to the Bravais group of the translation lattice, $\mathcal{B}(L)$, so that $(\boldsymbol{P}, \boldsymbol{p})$ is an isometry.

7.4.3 Translation part of Euclidean normalizer

Let $\boldsymbol{P}$ be an element of Bravais group $\mathcal{B}(L)$. If $(\boldsymbol{P}, \boldsymbol{p}) \in \mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$, the condition

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{G} \tag{61}$$

gives

$$(\boldsymbol{E} - \boldsymbol{W}')\boldsymbol{p} = \boldsymbol{w}' - \boldsymbol{P}\boldsymbol{w} \pmod{\mathbb{Z}^n} \quad (\forall (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}). \tag{62}$$

Conversely, a set of operations $(\boldsymbol{P}, \boldsymbol{p})$ satisfying Eq. (62) is a subgroup of $\mathcal{E}_n$.

8 Lattice computation

References: [14–17]

8.1 Lattice

8.1.1 Choice of basis vectors of lattice

The choice of basis vectors is not unique for a given lattice. A lattice spanned by basis vectors $(\boldsymbol{a}_1, \dots, \boldsymbol{a}_n)$ and a lattice spanned by

$$(\boldsymbol{a}'_1, \dots, \boldsymbol{a}'_n) \coloneqq (\boldsymbol{a}_1, \dots, \boldsymbol{a}_n)\boldsymbol{P} \quad (\boldsymbol{P} \in \mathbb{R}^{n \times n})$$

coincide if and only if $\boldsymbol{P} \in \mathrm{SL}(n, \mathbb{Z})$, where $\mathrm{SL}(n, \mathbb{Z})$ is the set of $n \times n$ unimodular matrices.

8.1.2 Delaunay reduction

8.2 Sublattice, Hermite normal form, and their applications

8.2.1 Sublattices and their equivalence

A *sublattice* is a subset of lattice L obtained by removing some lattice points from L[8]. A set of basis vectors of the sublattice is identified with the transformation matrix $\boldsymbol{M}$ such that the original set of basis vectors $\boldsymbol{A}$ is transformed into a new set of basis vectors $\boldsymbol{AM}$. Therefore, the sublattice $L_{\boldsymbol{M}}$ is the set of lattice points expressed as

$$L_{\boldsymbol{M}} = \left\{ \boldsymbol{AMn} \,\middle|\, \boldsymbol{n} \in \mathbb{Z}^3 \right\}. \tag{63}$$

We refer to the absolute value of the determinant of $\boldsymbol{M}$, $\det \boldsymbol{M}$, as the index of the sublattice $L_{\boldsymbol{M}}$. The index is identical to the number of lattice points in the sublattice $L_{\boldsymbol{M}}$.

8.2.2 Hermite normal form

Let $\boldsymbol{U}$ be a three-dimensional square unimodular matrix, where all elements are integers and $\det \boldsymbol{U} = \pm 1$. Two matrices $\boldsymbol{M}$ and $\boldsymbol{MU}$ are equivalent in terms of lattice transformation. This means that they derive the same sublattice expressed as

$$L_{\boldsymbol{M}} = L_{\boldsymbol{MU}}. \tag{64}$$

Their representative can be the canonical form called the *Hermite normal form* (HNF). Any transformation matrix $\mathbf{M}$ can be converted to a unique form of the lower-triangular integer matrix, HNF, by multiplying the unimodular matrix $\mathbf{U}'$ from the right

[8] In other fields than mathematics and crystallography, a substructure of a crystal structure is called a "sublattice", and a superstructure of a crystal structure is called a "superlattice".

satisfying the relationship

$$\mathbf{MU}' = \begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix}, \tag{65}$$

where $a > 0$, $0 \leq b < c$, $0 \leq d < f$, and $0 \leq e < f$. The requirement that diagonal elements a, c, and f are all positive eliminates equivalent basis vectors obtained by inversion. Also, the addition of a basis vector to another one or the subtraction of a basis vector from another one does not change the lattice itself. Thus, we can choose remainders of f as d and e, and a remainder of c as b.

Let us generalize HNFs to $m \times n$ integer matrix, $\boldsymbol{M}$. It has a (column-style) Hermite normal form $\boldsymbol{H}$ if there exists a unimodular matrices $\boldsymbol{R} \in \mathbb{Z}^{n\times n}$ such that $\boldsymbol{H} = \boldsymbol{MR}$ satisfied the following conditions

1. $H_{ij} \geq 0 \quad (1 \leq i \leq m, 1 \leq j \leq n)$
2. $H_{ij} = 0 \quad (i < j, j > r)$
3. $H_{ij} < H_{ii} \quad (i > j, 1 \leq i \leq r)$
4. $r = \mathrm{rank}\boldsymbol{M}$

If $\mathbf{M}$ is full rank, the Hermite normal form $\boldsymbol{H}$ is uniquely determined.

8.2.3 Example to compute HNF

8.2.4 Union of lattices

Just compute HNF!

8.2.5 Integer linear system

For given $\boldsymbol{A} \in \mathbb{Z}^{m\times n}$ and $\boldsymbol{b} \in \mathbb{Z}^m$, consider to solve integer linear system $\boldsymbol{Ax} = \boldsymbol{b}$ in $\boldsymbol{x} \in \mathbb{Z}^n$. Let the Hermite normal form of $\boldsymbol{A}$ be $\boldsymbol{H} = \boldsymbol{AR}$, where $\boldsymbol{R}$ is unimodular and $\boldsymbol{H}$ is lower triangular. The given linear system is

$$\begin{pmatrix} H_{11} & & \boldsymbol{O} & \vdots \\ \vdots & \ddots & & \boldsymbol{0} \\ H_{r1} & \dots & H_{rr} & \vdots \\ \dots & \boldsymbol{0} & \dots & \boldsymbol{O} \end{pmatrix} \boldsymbol{y} = \boldsymbol{b} \tag{66}$$

where $\mathbf{y} \coloneqq \boldsymbol{R}^{-1}\boldsymbol{x}$. A special solution, $\boldsymbol{x}_{\mathrm{special}} = \boldsymbol{R}\boldsymbol{y}_{\mathrm{special}}$, is determined by Gaussian elimination if exists. A general solution for $\boldsymbol{Hy} = \boldsymbol{0}$ is given by

$$\boldsymbol{y} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ n_{r+1} \\ \vdots \\ n_m \end{pmatrix} \quad (\forall n_{r+1}, \dots, n_m \in \mathbb{Z}). \tag{67}$$

8.3 Smith normal form and its applications

8.3.1 Distinct lattice points in sublattice

When we consider the translational symmetry of a sublattice $L_{\boldsymbol{M}}$, two lattice points $\boldsymbol{m}, \boldsymbol{m}$ are equivalent if the distance between the two lattice points is a translation of $L_{\boldsymbol{M}}$, that is,

$$\boldsymbol{m} - \boldsymbol{m}' \in \boldsymbol{M}\mathbb{Z}^3. \tag{68}$$

The SNF of the transformation matrix $\mathbf{M}$ is useful to concretely write down Eq. (68). The SNF is one of the decompositions of an integer matrix $\mathbf{M}$ as

$$\boldsymbol{S} = \boldsymbol{PMQ}, \tag{69}$$

where $\boldsymbol{P}$ and $\boldsymbol{Q}$ are unimodular matrices, and $\mathbf{S}$ is a diagonal integer matrix,

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}. \tag{70}$$

Here S_{11} is a divisor of S_{22}, and S_{22} is a divisor of S_{33}. We can rewrite Eq. (68) with Eq. (69) as

$$[\boldsymbol{Pm}]_{\boldsymbol{S}} = [\boldsymbol{Pm}']_{\boldsymbol{S}}, \tag{71}$$

where $[\cdot]_{\boldsymbol{S}}$ indicates to take modulus for the ith row by S_{ii}. We mention that the range of $[\cdot]_{\mathbf{S}}$ is $\mathbb{Z}_{S_{11}} \times \mathbb{Z}_{S_{22}} \times \mathbb{Z}_{S_{33}}$ because a value of the ith row is a remainder by S_{ii}.

8.3.2 Smith normal form

Let $\boldsymbol{M}$ be $m \times n$ integer matrix. There exist some unimodular matrices $\boldsymbol{L} \in \mathbb{Z}^{m \times m}$ and $\boldsymbol{R} \in \mathbb{Z}^{n \times n}$ such that

$$\boldsymbol{D} := \boldsymbol{LMR} = \begin{pmatrix} d_1 & & \boldsymbol{O} & \mathbf{0} \\ & \ddots & & \vdots \\ \boldsymbol{O} & & d_r & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \boldsymbol{O} \end{pmatrix}, \tag{72}$$

where d_i is positive integer and d_{i+1} devides d_i. Then $\boldsymbol{D}$ is called Smith normal form.

8.3.3 Extended Euclidean algorithm

https://twitter.com/tmaehara/status/1431205927353528321

8.3.4 Procedure to compute SNF

$$\begin{aligned}
\begin{pmatrix} 2 & 4 & 4 \\ -6 & 6 & 12 \\ 10 & -4 & -16 \end{pmatrix} &\to \begin{pmatrix} 2 & 0 & 0 \\ -6 & 18 & 24 \\ 10 & -24 & -36 \end{pmatrix} \to \begin{pmatrix} 2 & 0 & 0 \\ 0 & 18 & 24 \\ 0 & -24 & -36 \end{pmatrix} \\
&\to \begin{pmatrix} 2 & 0 & 0 \\ 0 & 18 & 6 \\ 0 & -24 & -12 \end{pmatrix} \to \begin{pmatrix} 2 & 0 & 0 \\ 0 & 18 & 6 \\ 0 & 12 & 0 \end{pmatrix} \\
&\to \begin{pmatrix} 2 & 0 & 0 \\ 0 & 6 & 18 \\ 0 & 0 & 12 \end{pmatrix} \to \begin{pmatrix} 2 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 12 \end{pmatrix}
\end{aligned}$$

8.3.5 Frobenius congruent

For given $\boldsymbol{A} \in \mathbb{Z}^{m \times n}$ and $\boldsymbol{b} \in \mathbb{Z}^m$, consider to solve Frobenius congruent $\boldsymbol{Ax} \equiv \boldsymbol{b} \pmod{\mathbb{R}/\mathbb{Z}}$ for $\boldsymbol{x} \in \mathbb{R}^n$. Let SNF of $\boldsymbol{A}$ be $\boldsymbol{D} = \boldsymbol{LAR}$, where $\boldsymbol{L}$ and $\boldsymbol{R}$ are unimodular matrices.

$$\boldsymbol{LAx} = \boldsymbol{Lb} + \mathbb{Z}^n \tag{73}$$

$$\boldsymbol{Dy} = \boldsymbol{v} + \mathbb{Z}^n \quad \text{where}\, \boldsymbol{y} := \boldsymbol{R}^{-1}\boldsymbol{x},\, \boldsymbol{v} := \boldsymbol{Lb} \tag{74}$$

$$\boldsymbol{y} = \begin{pmatrix} \frac{v_1}{D_{11}} \\ \vdots \\ \frac{v_r}{D_{rr}} \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{D_{11}} n_1 \\ \vdots \\ \frac{1}{D_{rr}} n_r \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{r+1} \\ \vdots \\ a_m \end{pmatrix} \quad (\forall n_1, \dots, n_r \in \mathbb{Z}, \forall a_{r+1}, \dots, a_m \in \mathbb{R}) \tag{75}$$

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