Crystal Symmetry Primer*

Kohei Shinohara†

February 27, 2023

Contents

†https://lan496.github.io/

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 $\mathbf{A} \coloneqq (\mathbf{a}_1, \cdots, \mathbf{a}_n)$ 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 $\boldsymbol{P}^\top \boldsymbol{G} \boldsymbol{P}$.

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 $\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n$.

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

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

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

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

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

[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 $\begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix}$ 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.

1.2 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

$$
\mathcal{E}_n := \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \,\middle|\, \boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G}, \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{12}
$$

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

$$
\mathcal{T}_n := \left\{ \begin{pmatrix} \boldsymbol{I}_n & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \,\middle|\, \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{13}
$$

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.

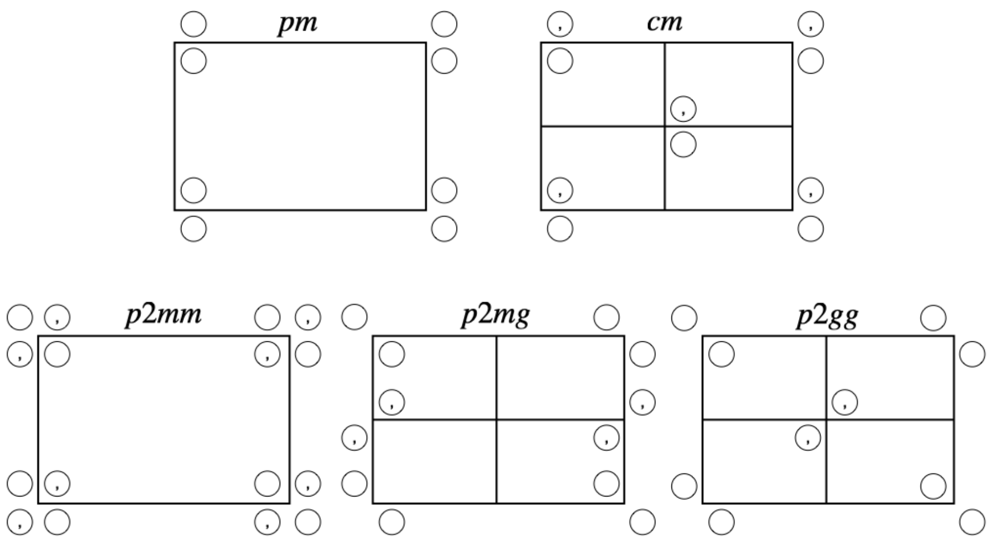


Figure 1: Example diagrams of plane groups

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].

[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.

The plane group cm is generated by the matrices

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

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

2.1 Definition

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

$$\begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{W}_2 & \boldsymbol{w}_2 \\ \boldsymbol{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}_1 \boldsymbol{W}_2 & \boldsymbol{W}_1 \boldsymbol{w}_2 + \boldsymbol{w}_1 \\ \boldsymbol{0}^T & 1 \end{pmatrix} \in \mathcal{A}_n. \tag{14}$$

The inverse of an affine mapping is also an affine mapping,

$$\begin{pmatrix} \boldsymbol{W}_1 & \boldsymbol{w}_1 \\ \boldsymbol{0}^T & 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{W}_1^{-1} & -\boldsymbol{W}_1^{-1} \boldsymbol{w}_1 \\ \boldsymbol{0}^T & 1 \end{pmatrix} \in \mathcal{A}_n. \tag{15}$$

TODO: generator

2.2 Abelian group

translation subgroup

2.3 Isomorphism, subgroup

TODO: Euclidean group is a subgroup of the affine group.

2.4 Coset decomposition, normal subgroup, factor group

TODO: Translation subgroup is a normal subgroup of a space group

$\mathbb{Z}_2$ in $\mathbb{Z}_4$

2.5 Homomorphism, kernel, image

point group

2.6 Conjugation

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 $\mathcal{E}_n$

$$\mathcal{G} := \mathrm{Stab}_{\mathcal{E}_n}(f) = \{g \in \mathcal{E}_n \mid g \cdot f = f\} \tag{16}$$

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 $\mathcal{G}$.

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

$$(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{I}_n, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w})^{-1} = (\boldsymbol{I}_n, \boldsymbol{W}\boldsymbol{t}) \in \mathcal{T}(\mathcal{G}). \tag{17}$$

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

$$\mathcal{P} := \{\mathbf{W} \mid (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}\}. \tag{18}$$

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

We fix some basis vectors $(\boldsymbol{a}_1, \dots, \boldsymbol{a}_n)$ of affine space, and act all mappings in $\mathcal{P}$ on the basis vectors. Since mapping in the point group $\mathcal{P}$ is an 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 $\max_{i=1,\cdots,n} \mathbf{a}_i$.

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 Vector system

In general, a space group is not specified only with a point group and translation subgroup. We need to determine a translation part of each symmetry operation.

Definition 3.4 (vector system)**.** 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*:

$$\boldsymbol{\tau}(gh) = g\boldsymbol{\tau}(h) + \boldsymbol{\tau}(g) \pmod{\mathbb{Z}^n} \quad (\forall g, h \in \mathcal{P}). \tag{19}$$

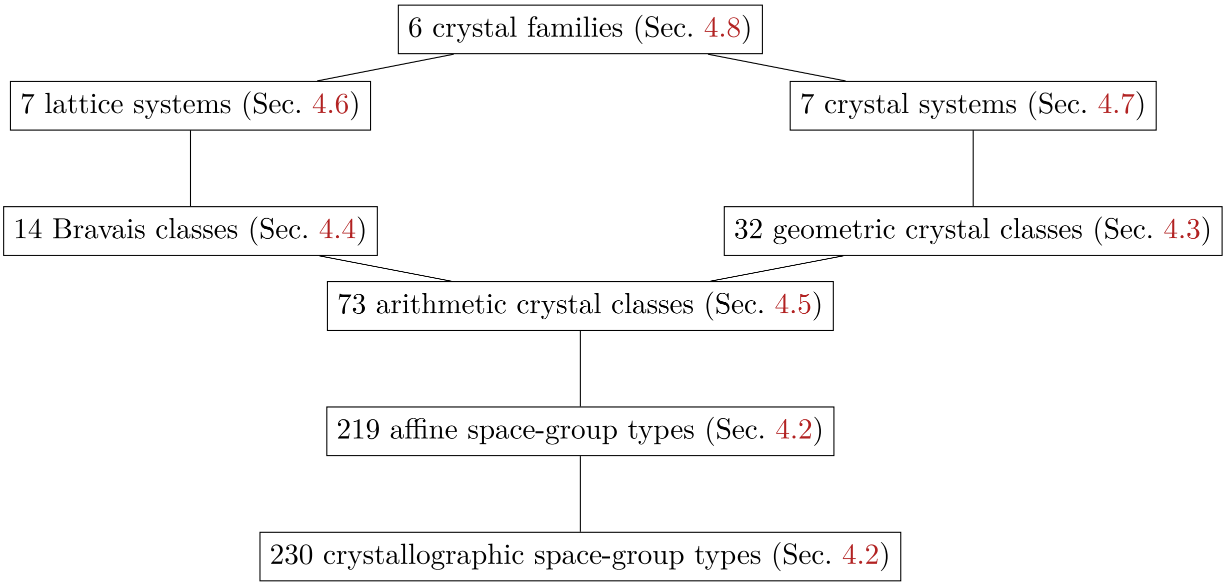
We remark that we require the cocycle condition to have a vector system consistent with the product of two symmetry operations,

$$\begin{pmatrix} g & \boldsymbol{\tau}(g) \\ \mathbf{0}^\top & 1 \end{pmatrix} \begin{pmatrix} h & \boldsymbol{\tau}(h) \\ \mathbf{0}^\top & 1 \end{pmatrix} = \begin{pmatrix} gh & g\boldsymbol{\tau}(h) + \boldsymbol{\tau}(g) \\ \mathbf{0}^\top & 1 \end{pmatrix}$$

TODO: symmorphic and nonsymmorphic space groups

3.4 Working examples from plane groups

4 Classification of space groups



We classify space groups in three dimensions.

4.1 Transformation matrix, origin shift

When we change the origin and basis vectors for the affine space from O and $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)$ to $\boldsymbol{p}$ and $(\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3)\boldsymbol{P}$, the components of point coordinates and affine mappings are also changed as follows.

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

$$\begin{aligned} \boldsymbol{x}' &= (\boldsymbol{P}, \boldsymbol{p})^{-1}\boldsymbol{x} \\ &= \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p}). \end{aligned} \tag{20}$$

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

$$\begin{aligned} (\boldsymbol{W}', \boldsymbol{w}') &= (\boldsymbol{P}, \boldsymbol{p})^{-1}(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p}) \\ &= \left(\boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P}, \boldsymbol{P}^{-1}(\boldsymbol{W}\boldsymbol{p} + \boldsymbol{w} - \boldsymbol{p})\right). \end{aligned} \tag{21}$$

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

$$\boldsymbol{G}' = \boldsymbol{P}^\top \boldsymbol{G} \boldsymbol{P}. \tag{22}$$

4.2 Affine space-group type and space-group type

It is natural to identify two space groups that are transformed into the 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,

$$\exists (\boldsymbol{P}, \boldsymbol{p}) \in \mathcal{A}_3 \quad s.t. \quad (\boldsymbol{P}, \boldsymbol{p})^{-1} \mathcal{G} (\boldsymbol{P}, \boldsymbol{p}) = \mathcal{G}'. \tag{23}$$

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 [4].

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,

$$\exists (\boldsymbol{P}, \boldsymbol{p}) \in \mathcal{A}_3^+ \quad s.t. \quad (\boldsymbol{P}, \boldsymbol{p})^{-1} \mathcal{G} (\boldsymbol{P}, \boldsymbol{p}) = \mathcal{G}', \tag{24}$$

where orientation-preserving affine mapping is an affine mapping whose linear part is positive,

$$\mathcal{A}_n^+ := \left\{ \begin{pmatrix} \boldsymbol{W} & \boldsymbol{w} \\ \boldsymbol{0}^\top & 1 \end{pmatrix} \middle| \, \boldsymbol{W} \in \mathrm{GL}(n, \mathbb{R}), \det \boldsymbol{W} > 0, \boldsymbol{w} \in \mathbb{R}^n \right\}. \tag{25}$$

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. 1.

4.3 Geometric crystal class

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

[4] 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.

Table 1: 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)

Table 2: 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, $\overline{4}32$, $m\overline{3}m$

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,

$$\exists \boldsymbol{P} \in \mathrm{GL}(3, \mathbb{R}) \quad s.t. \quad \boldsymbol{P}^{-1} \mathcal{P} \boldsymbol{P} = \mathcal{P}'. \tag{26}$$

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.

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 2).

TODO: $3m1$ and $31m$

4.4 Bravais type of lattice and Bravais class

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 $\mathcal{G}$,

$$L = \{\boldsymbol{t} \mid (\boldsymbol{I}_3, \boldsymbol{t}) \in \mathcal{G}\}. \tag{27}$$

Definition 4.6 (Bravais group)**.** A set of isometry mapping that pertains L is called *Bravais group of* L. Letting $\boldsymbol{G}$ be a metric tensor of L, Bravais group of L is

$$\mathcal{B}(L) \coloneqq \left\{\boldsymbol{W} \in \mathrm{GL}(3,\mathbb{Z}) \,\middle|\, \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G}\right\}. \tag{28}$$

We mention that a 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,

$$\exists \boldsymbol{P} \in \mathrm{SL}(3,\mathbb{Z}) \quad s.t. \quad \boldsymbol{P}^{-1}\mathcal{B}(L)\boldsymbol{P} = \mathcal{B}(L'). \tag{29}$$

Remarkably, this definition of Bravais types of lattices is independent of choices for primitive basis.

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,

$$\boldsymbol{M}(K) \coloneqq \left\{\boldsymbol{G} \in \mathbb{R}^{3\times 3}_{\mathrm{sym}} \,\middle|\, \boldsymbol{W}^\top \boldsymbol{G} \boldsymbol{W} = \boldsymbol{G} \quad (\forall \boldsymbol{W} \in K)\right\} \tag{30}$$

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*.

TODO: Add example of specialized metric and Euclidean normalizer

Definition 4.9 (Bravais class)**.** Let L be a lattice with a metric tensor $\boldsymbol{G}$. A space group $\mathcal{G}$ with a point group $\mathcal{P}$ and a translation lattice L 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 in $\mathrm{SL}(3,\mathbb{Z})$,

$$\exists \boldsymbol{P} \in \mathrm{SL}(3,\mathbb{Z})\, s.t.\, \boldsymbol{P}^{-1}\boldsymbol{M}(\mathcal{P})\boldsymbol{P} = \boldsymbol{M}(\mathcal{B}(L)). \tag{31}$$

TODO: 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 $\mathcal{P}$.

TODO: limiting case from mP to oS

4.5 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,

$$\exists \boldsymbol{P} \in \mathrm{SL}(3,\mathbb{R}) \quad s.t. \quad \boldsymbol{P}^{-1}\mathcal{P}\boldsymbol{P} = \mathcal{P}'. \tag{32}$$

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

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 $\mathcal{G}$,

$$\mathcal{P} = \mathcal{B}(L). \tag{33}$$

Note that Bravais arithmetic crystal classes are classifications for arithmetic crystal classes of space groups, and Bravais classes are classifications for space groups. The definition of Bravais arithmetic crystal classes is compatible with that of Bravais types of lattices (see Table 3).

TODO: Example: cm and pm

4.6 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,

$$\exists \boldsymbol{P} \in \mathrm{SL}(3,\mathbb{Z})\, s.t.\, \boldsymbol{P}^{-1}\mathcal{B}(L)\boldsymbol{P} = \mathcal{B}(L'). \tag{34}$$

TODO: definition of lattice system on space groups

Table 4

Table 3: The correspondence of Bravais arithmetic crystal classes and Bravais types of lattices in three dimensions.

Bravais type of lattice	Bravais arithmetic crystal class
aP	$\overline{1}P$ (2)
mP	$2/mP$ (10)
mC	$2/mC$ (12)
oP	$mmmP$ (47)
oS	$mmmC$ (65)
oF	$mmmF$ (69)
oI	$mmmI$ (71)
tP	$4/mmmP$ (123)
tI	$4/mmmI$ (139)
hR	$\overline{3}mR$ (166)
hP	$6/mmmP$ (191)
cP	$m\overline{3}mP$ (221)
cF	$m\overline{3}mF$ (225)
cI	$m\overline{3}mI$ (229)

Table 4: Lattice systems in space groups

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

4.7 Crystal system

TODO:

Two point groups belong to the same crystal system if and only if the sets of Bravais type of lattices on which these point groups act coincide.

Table 5

4.8 Crystal family

Table 5: 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	$m\overline{3}m, \overline{4}3m, 432, m\overline{3}, 23$

Table 6: 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	$\langle 001\rangle = [100][010][001]$	$\langle 111\rangle = [111][1\bar{1}\bar{1}][\bar{1}11][\bar{1}\bar{1}1]$	$\langle 110\rangle = [1\bar{1}0][110][01\bar{1}][011][\bar{1}01][101]$

Table 7: settings of monoclinic system

unique axis setting	$\mathbf{b}$ $\mathbf{a}\underline{\mathbf{b}}\mathbf{c}$	$-\mathbf{b}$ $\mathbf{c}\underline{\bar{\mathbf{b}}}\mathbf{a}$	$\mathbf{c}$ $\mathbf{ab}\underline{\mathbf{c}}$	$-\mathbf{c}$ $\mathbf{ba}\underline{\bar{\mathbf{c}}}$	$\mathbf{a}$ $\underline{\mathbf{a}}\mathbf{bc}$	$-\mathbf{a}$ $\underline{\bar{\mathbf{a}}}\mathbf{bc}$
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	$I \to I$	$I \to I$	$I \to I$	$I \to I$	$I \to I$	$I \to I$

5 Conventions for space groups

5.1 Conventional cell

5.2 Helmann–Mauguin symbol

Convention for Hermann-Mauguin symbols is shown in Table 6.

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 7. Cell choices for monoclinic systems are shown in Table 8 and Fig. 2.

Table 8: 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	$C \to C$	$A \to C$	$I \to C$

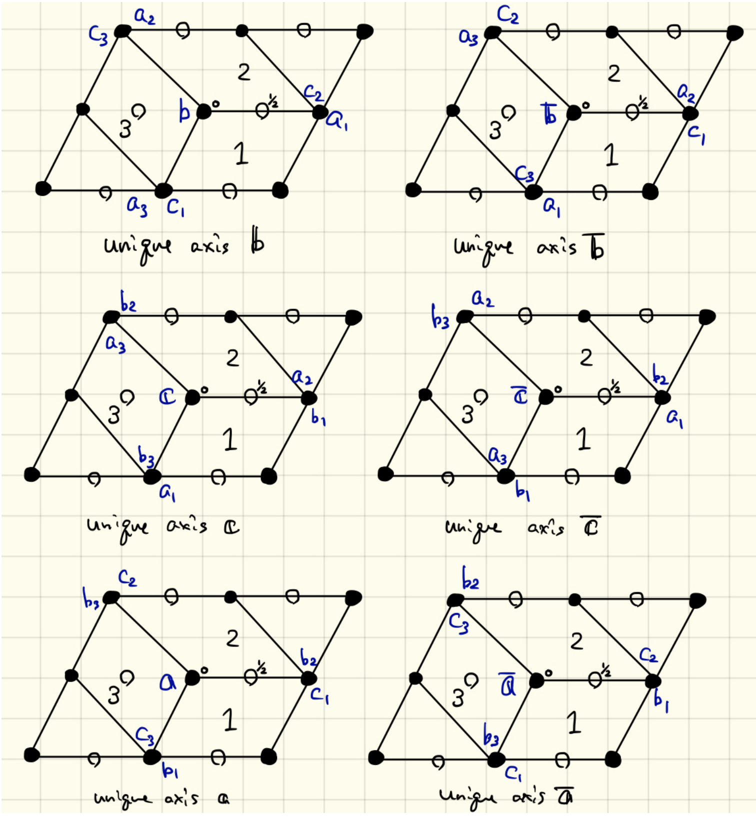


Figure 2: choices of monoclinic system

5.3.2 Orthorhombic system

Axis settings for orthorhombic systems are shown in Table 9.

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 9: 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

$$\mathcal{T}(\mathcal{M}) \coloneqq \{(\boldsymbol{E}, \boldsymbol{t}) \mid \exists \theta \in \{1, 1'\}, (\boldsymbol{E}, \boldsymbol{t})\theta \in \mathcal{M}\}\,. \tag{35}$$

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

$$\mathcal{P}(\mathcal{M}) \coloneqq \left\{\boldsymbol{W}\theta \,\middle|\, \exists \boldsymbol{w} \in \mathbb{R}^3, (\boldsymbol{W}, \boldsymbol{w})\theta \in \mathcal{M}\right\}. \tag{36}$$

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:

$$\mathcal{F}(\mathcal{M}) \coloneqq \{(\boldsymbol{W}, \boldsymbol{w}) \mid \exists \theta \in \{1, 1'\}, (\boldsymbol{W}, \boldsymbol{w})\theta \in \mathcal{M}\}\,. \tag{37}$$

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

$$\mathcal{D}(\mathcal{M}) \coloneqq \{(\boldsymbol{W}, \boldsymbol{w}) \mid (\boldsymbol{W}, \boldsymbol{w})1 \in \mathcal{M}\}\,. \tag{38}$$

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 *klessengleiche* 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 [7]. 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 Action, orbit, stabilizer

7.2 Site symmetry group, Wyckoff position, asymmetric unit

7.3 Euclidean normalizer and affine normalizer

7.4 Wyckoff set, equivalent descriptions of crystal structure

7.5 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

$$\det \boldsymbol{P} \neq 0 \tag{39}$$

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{W}', \boldsymbol{w}'), \tag{40}$$

where

$$\boldsymbol{W}' = \boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{-1} \tag{41}$$

$$\boldsymbol{w}' = \boldsymbol{p} + \boldsymbol{P}\boldsymbol{w} - \boldsymbol{P}\boldsymbol{W}\boldsymbol{P}^{-1}\boldsymbol{p}. \tag{42}$$

7.5.1 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

$$\boldsymbol{W}' = \boldsymbol{W} \tag{43}$$

$$\boldsymbol{w}' = \boldsymbol{p} + \boldsymbol{w} - \boldsymbol{W}\boldsymbol{p}. \tag{44}$$

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

$$(\boldsymbol{W}, \boldsymbol{w}')^{-1}(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{E}, \boldsymbol{w} - \boldsymbol{w}') \in \mathcal{S}. \tag{45}$$

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

$$(\boldsymbol{E} - \boldsymbol{W})\boldsymbol{p} = \mathbf{0} (\mathrm{mod}\, \mathbb{Z}^n) \tag{46}$$

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

Conversely, a set of operations $(\boldsymbol{E}, \boldsymbol{p})$ satisfying Eq. (46) is a subgroup of $\mathrm{Stab}_{\mathcal{E}_n}(\mathcal{G})$.

The linear integer system of Eq. (46) 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.

7.5.2 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

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{E}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{E}, \boldsymbol{P}\boldsymbol{w}) \in \mathcal{G}. \tag{47}$$

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.

7.5.3 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

$$(\boldsymbol{P}, \boldsymbol{p})(\boldsymbol{W}, \boldsymbol{w})(\boldsymbol{P}, \boldsymbol{p})^{-1} = (\boldsymbol{W}', \boldsymbol{w}') \in \mathcal{G} \tag{48}$$

gives

$$(\boldsymbol{E} - \boldsymbol{W}')\boldsymbol{p} = \boldsymbol{w}' - \boldsymbol{P}\boldsymbol{w} \pmod{\mathbb{Z}^n} \quad (\forall (\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{G}). \tag{49}$$

Conversely, a set of operations $(\boldsymbol{P}, \boldsymbol{p})$ satisfying Eq. (49) is a subgroup of $\mathcal{E}_n$.

8 Lattice computation

References: [8–11]

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 $(\boldsymbol{a}_1, \ldots, \boldsymbol{a}_n)$ and a lattice spanned by

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

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 [5]. 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

$$L_{\boldsymbol{M}} = \left\{ \boldsymbol{AMn} \,\middle|\, \boldsymbol{n} \in \mathbb{Z}^3 \right\}. \tag{50}$$

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

$$L_{\boldsymbol{M}} = L_{\boldsymbol{MU}}. \tag{51}$$

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

[5] 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

$$\mathbf{M}\mathbf{U}' = \begin{pmatrix} a & 0 & 0 \\ b & c & 0 \\ d & e & f \end{pmatrix}, \tag{52}$$

where $a > 0$, $0 \le b < c$, $0 \le d < f$, and $0 \le e < f$. 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. $H_{ij} \ge 0 \quad (1 \le i \le m, 1 \le j \le n)$
2. $H_{ij} = 0 \quad (i < j, j > r)$
3. $H_{ij} < H_{ii} \quad (i > j, 1 \le i \le r)$
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

$$\begin{pmatrix} H_{11} & & \boldsymbol{O} & \vdots \\ \vdots & \ddots & & \mathbf{0} \\ H_{r1} & \dots & H_{rr} & \vdots \\ \dots & \mathbf{0} & \dots & \boldsymbol{O} \end{pmatrix} \boldsymbol{y} = \boldsymbol{b} \tag{53}$$

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

$$\boldsymbol{y} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ n_{r+1} \\ \vdots \\ n_m \end{pmatrix} \quad (\forall n_{r+1}, \cdots, n_m \in \mathbb{Z}). \tag{54}$$

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,

$$\boldsymbol{m} - \boldsymbol{m}' \in \boldsymbol{M}\mathbb{Z}^3. \tag{55}$$

The SNF of the transformation matrix $\mathbf{M}$ is useful to concretely write down Eq. (55). The SNF is one of the decompositions of an integer matrix $\mathbf{M}$ as

$$\boldsymbol{S} = \boldsymbol{P}\boldsymbol{M}\boldsymbol{Q}, \tag{56}$$

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

$$\boldsymbol{S} = \begin{pmatrix} S_{11} & 0 & 0 \\ 0 & S_{22} & 0 \\ 0 & 0 & S_{33} \end{pmatrix}. \tag{57}$$

Here S_{11} is a divisor of S_{22}, and S_{22} is a divisor of S_{33}. We can rewrite Eq. (55) with Eq. (56) as

$$[\boldsymbol{P}\boldsymbol{m}]_{\boldsymbol{S}} = [\boldsymbol{P}\boldsymbol{m}']_{\boldsymbol{S}}, \tag{58}$$

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

$$\boldsymbol{D} \coloneqq \boldsymbol{L}\boldsymbol{M}\boldsymbol{R} = \begin{pmatrix} d_1 & & \boldsymbol{O} & \mathbf{0} \\ & \ddots & & \vdots \\ \boldsymbol{O} & & d_r & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \boldsymbol{O} \end{pmatrix}, \tag{59}$$

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 $\boldsymbol{Ax} \equiv \boldsymbol{b} \,(\mathrm{mod}\, \mathbb{R}/\mathbb{Z})$ 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.

$$\boldsymbol{LAx} = \boldsymbol{Lb} + \mathbb{Z}^n \tag{60}$$

$$\boldsymbol{Dy} = \boldsymbol{v} + \mathbb{Z}^n \quad \text{where}\, \boldsymbol{y} := \boldsymbol{R}^{-1}\boldsymbol{x},\ \boldsymbol{v} := \boldsymbol{Lb} \tag{61}$$

$$\boldsymbol{y} = \begin{pmatrix} \frac{v_1}{D_{11}} \\ \vdots \\ \frac{v_r}{D_{rr}} \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \begin{pmatrix} \frac{1}{D_{11}} n_1 \\ \vdots \\ \frac{1}{D_{rr}} n_r \\ 0 \\ \vdots \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{r+1} \\ \vdots \\ a_m \end{pmatrix} \quad (\forall n_1, \cdots, n_r \in \mathbb{Z}, \forall a_{r+1}, \cdots, a_m \in \mathbb{R}) \tag{62}$$

References

[1] M. I. Aroyo, editor. *International Tables for Crystallography*, volume A. International Union of Crystallography, December 2016.

[2] 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.

[3] Bernd Souvignier. Group theory applied to crystallography. https://www.math.ru.nl/~souvi/krist_09/cryst.pdf.

[4] Ulrich Müller. *Symmetry relationships between crystal structures: applications of crystallographic group theory in crystal chemistry*, volume 18. OUP Oxford, 2013.

[5] Michael Glazer, Gerald Burns, and Alexander N Glazer. *Space groups for solid state scientists.* Elsevier, 2012.

[6] Commission for Crystallographic Nomenclature of the International Union of Crystallography. Online dictionary of crystallography. https://dictionary.iucr.org/Main_Page.

[7] N. V. Belov, N. N. Neronova, and T. S. Smirnova. Shubnikov groups. *Sov. Phys. Crystallogr.*, 2:311–322, 1957.

[8] Gus L. W. Hart and Rodney W. Forcade. Algorithm for generating derivative structures. *Phys. Rev. B*, 77:224115, Jun 2008.

[9] Gus L. W. Hart and Rodney W. Forcade. Generating derivative structures from multilattices: Algorithm and application to hcp alloys. *Phys. Rev. B*, 80:014120, Jul 2009.

[10] Henri Cohen. *A Course in Computational Algebraic Number Theory.* Springer Berlin Heidelberg, 1993.

[11] Daniele Micciancio. Cse206a: Lattices algorithms and applications (winter 2010). https://cseweb.ucsd.edu/classes/wi10/cse206a/.