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

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 Symmetry operation, isometry

1.2 Affine group, Euclidean group

1.3 Matrix-column pair, Setiz symbol, augmented matrix, short-hand notation

Note: hexagonal axis for $p3$

1.4 Screw and glide

1.5 Working example from plane group

2 Group theory primer

2.1 Definition

2.2 Abelian group

translation subgroup

2.3 Isomorphism, subgroup

2.4 Coset decomposition, normal subgroup, factor 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

3.2 Point group

3.3 Vector system

symmorphic and nonsymmorphic space groups

3.4 Working example from plane group

4 Classification of space groups

4.1 Transformation matrix, origin shift

4.2 219 affine space-group types

4.3 230 space-group types

11 enantiomorphic pairs

4.4 32 geometric crystal classes

4.5 14 Bravais types of lattices

limiting case
    special metric

4.6 7 crystal systems

4.7 73 arithmetic crystal classes

5 Conventions for space groups

5.1 Conventional cell

5.2 Helmann–Mauguin symbol

Principal directions

How to read H-M symbols

5.3 Standard settings in ITA

5.4 Hall symbol

6 Magnetic space group

6.1 Definition

6.2 BNS and OG symbols

6.3 Construction type of magnetic space group

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

7.4 Wyckoff set, equivalent descriptions of crystal structure

7.5 Affine normalizer

8 Lattice computation

8.1 Delaunay reduction

8.2 Choice of basis vectors, sublattice

8.3 Hermite normal form

8.4 Smith normal form

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.