Space Groups

Internal Symmetry of Crystals

Fractional Coordinates

• We describe the position of any atom within the unit cell in terms of fractions of the unit cell edge.
  – The corner is thus (0, 0, 0)
  – The center is (.5, .5, .5)
• The symmetry operations will then repeat atoms within the box.

Space Groups

• If translation operations are included with rotation and inversion,
• We have 230 three-dimensional space groups.
• Translation operations
  – Unit cell translations
  – Centering operations (Lattices) (A, B, C, I, F, R)
  – Glide planes (reflection + translation) (a, b, c, n, d)
  – Screw axes (rotation + translation) (21, 31, 32)

Lattices (centering operations)

• A symmetry operation within the unit cell that generates equivalent atom positions within the cell.

Fractional Coordinates

Lattices (centering operations)

• P is for primitive
  – No centering operation

Space Groups

• 230 three-dimensional space groups
• Hermann-Mauguin symbols. (4 positions)
• First position is Lattice type (P, A, B, C, I, F or R)
• Second, third and fourth positions as with point groups

Lattices (centering operations)
**Lattices**

- **A, B, and C are end-centered**

  - A: for any atom at x, y, z, there is an identical atom at x, 0.5+y, 0.5+z
  - B: for any atom at x, y, z, there is an identical atom at 0.5+x, y, 0.5+z
  - C: for any atom at x, y, z, there is an identical atom at 0.5+x, 0.5+y, z

**Lattices**

- **A**, **B**, and **C**

  - A: (0, 0.5, 0.5)
  - B: (0.5, 0, 0.5)
  - C: (0.5, 0.5, 0)

**Lattices**

- **I is body-centered**
  - Point @ (0.5, 0.5, 0.5)
  - Multiplicity = 2

- **F is face-centered**
  - 0.5, 0.5, 0
  - 0.5, 0, 0.5
  - 0, 0.5, 0.5
  - Multiplicity = 4

**Lattices**

- **R is rhombohedral**
  - (2/3, 1/3, 1/3)
  - (1/3, 2/3, 2/3)
  - Multiplicity = 3
  - Trigonal system

**Rotation + Translation: Screw Diads**

- **2₁** is a 180° rotation plus ½ cell translation.

**Screw Triads**

- **3₁** is a 120° rotation plus a 1/3 cell translation.
- **3₂** is a 120° rotation plus a 2/3 cell translation.
**Screw Tetrads**

- 4₁ is a 90° rotation plus a 1/4 cell translation (right-handed).
- 4₂ is a 180° rotation plus a 1/2 cell translation (no handedness).
- 4₃ is a 90° rotation plus a 3/4 cell translation (left-handed).

**Glide Planes**

- Reflection plus 1/2 cell translation
  - a-glide: a/2 translation
  - b-glide: b/2 translation
  - c-glide: c/2 translation
  - n-glide (normal to a): b/2+c/2 translation
  - n-glide (normal to b): a/2+c/2 translation
  - n-glide (normal to c): a/2+b/2 translation
  - d-glide (tetragonal + cubic systems)

**Screw Hexads**

- 6₁ is a 60° rotation plus a 1/6 cell translation (right-handed).
- 6₂ is a 120° rotation plus a 1/3 cell translation (right-handed).
- 6₃ is a 180° rotation plus a 1/2 cell translation (no handedness).
- 6₄ is a 240° rotation plus a 2/3 cell translation (left-handed).
- 6₅ is a 300° rotation plus a 5/6 cell translation (left-handed).

**Glide Planes**

- Reflection plus 1/2 cell translation
  - a-glide: a/2 translation
  - b-glide: b/2 translation
  - c-glide: c/2 translation
  - n-glide (normal to a): b/2+c/2 translation
  - n-glide (normal to b): a/2+c/2 translation
  - n-glide (normal to c): a/2+b/2 translation
  - d-glide (tetragonal + cubic systems)

**Space Group Symmetry Diagrams**

- a-vertical
- b-horizontal
- c-normal to page
Space Group Symmetry Diagrams

- **Axis**
  - a 2 b
  - b 2 c
  - c 2 n

- **Plane**
  - \( P 21b 2a 2n = Pban \)

Pbcn

- **General**
  - (x, y, z)
  - (-x, -y, -z)
  - (x, -y, 1/2 + z)
  - (-x, y, 1/2 - z)
  - (1/2 - x, 1/2 + y, z)
  - (1/2 + x, 1/2 - y, -z)
  - (1/2 - x, 1/2 - y, 1/2 + z)
  - (1/2 + x, 1/2 + y, 1/2 - z)

- **Special**
  - (0, 0, 0)
  - (0, 0, 0)
  - (0, 0, 0.5)
  - (0, 0, 0.5)
  - (0.5, 0.5, 0)
  - (0.5, 0.5, 0)
  - (0.5, 0.5, 0.5)
  - (0.5, 0.5, 0.5)
**Enstatite Pbcn**

- Cell: $a=9.306; b=8.892; c=5.349\ \AA$
  - Mg1: $(0, 0.1006, 0.25)$
  - Mg2: $(0, 0.2625, 0.25)$
  - Si: $(0.2928, 0.0897, 0.0739)$
  - O1: $(0.1200, 0.0942, 0.0770)$
  - O2: $(0.3773, 0.2463, 0.0677)$
  - O3: $(0.3481, 0.9836, 0.3079)$

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**Quartz P3_121**

- Cell: $a=b=4.9137; c=5.4047\ \AA$
  - Si: $(0.4697, 0.0, 0.0)$
  - O: $(0.4133, 0.2672, 0.1188)$