Symmetry, Groups and Crystal Structures

The Seven Crystal Systems:
Ordered Atomic Arrangements

Crystal Morphology

- A face is designated by Miller indices in parentheses, e.g. (100) (111) etc.
- A form is a face plus its symmetric equivalents (in curly brackets) e.g. \{100\}, \{111\}.
- A direction in crystal space is given in square brackets e.g. [100], [111].

Halite Cube \{1 0 0\}

Fluorite Octahedra \{1 1 1\}
**Muscovite Cleavage**
*(0 0 1) c-axis perpendicular*

**Miller Indices**
- The cube face is (100)
- The cube form {100} comprises faces (100), (010), (001), (-100), (0-10), (00-1)

**Miller Indices: Clicker**
- A crystal face cuts the a axis at 2, the b axis at 3, and the c axis at 4. Its Miller Indices are:
  - A (2 3 4)
  - B (6 4 3)
  - C (1 4 3)
  - D (.5 .33 .25)
  - E (1 1 1)

**Halite Cube {100}**

**Stereographic Projections**
- Used to display crystal morphology.
- X for upper hemisphere.
- O for lower.

**Point Groups (Crystal Classes)**
- We can do symmetry operations in two dimensions or three dimensions.
- We can include or exclude the translation operations.
- Combining proper and improper rotation gives the point groups (Crystal Classes)
  - 32 possible combinations in 3 dimensions
  - 32 Crystal Classes (Point Groups)
  - Each belongs to one of the (seven) Crystal Systems
Space Groups

- Including the translation operations gives the space groups.
  - 17 two-dimensional space groups
  - 230 three dimensional space groups
- Each space group belongs to one of the 32 Crystal Classes (remove translations)

Groups

- The elements of our groups are symmetry operators.
- The rules limit the number of groups that are valid combinations of symmetry operators.
- The order of the group is the number of elements.

Minerals structures are described in terms of the unit cell

Learning Goals

- Describe a unit cell of a mineral, and draw a diagram of how it is defined (label cell edges (or axes) and inter-axial angles).
- List the seven crystal systems and describe their unit cell constraints.
- Distinguish 1-fold, 2-fold, 3-fold, 4-fold, and 6-fold rotations in two dimensions, and list the angles of rotation for each.

The Unit Cell

- The unit cell of a mineral is the smallest divisible unit of mineral that possesses all the symmetry and properties of the mineral.
- It is a small group of atoms arranged in a “box” with parallel sides that is repeated in three dimensions to fill space.
- It has three principal axes (a, b and c) and
- Three inter-axial angles (α, β, and γ)

The Unit Cell

- Three unit cell vectors a, b, c (Å)
- Three angles between vectors: α, β, γ (°)
  - α is angle between b and c
  - β is angle between a and c
  - γ is angle between a and b
Which angle is shown here?
1. $\alpha$
2. $\beta$
3. $\gamma$

Seven Crystal Systems

- The presence of symmetry operators places constraints on the geometry of the unit cell.
- The different constraints generate the seven crystal systems.
  - Triclinic
  - Monoclinic
  - Orthorhombic
  - Tetragonal
  - Trigonal
  - Hexagonal
  - Cubic (Isometric)

Quartz Unit Cell
$a = 4.914; b = 4.914; c = 5.405\text{Å}$
$\alpha = 90^\circ; \beta = 90^\circ; \gamma = 120^\circ$;

A. Triclinic
B. Monoclinic
C. Orthorhombic
D. Trigonal / Hexagonal
E. Cubic

Albite Unit Cell
$a = 8.137; b = 12.787; c = 7.157\text{Å}$
$\alpha = 94.24^\circ; \beta = 116.61^\circ; \gamma = 87.81^\circ$;

A. Triclinic
B. Monoclinic
C. Orthorhombic
D. Trigonal / Hexagonal
E. Cubic

Garnet Unit Cell
$a = 11.439; b = 11.439; c = 11.439\text{Å}$
$\alpha = 90^\circ; \beta = 90^\circ; \gamma = 90^\circ$;

A. Triclinic
B. Monoclinic
C. Orthorhombic
D. Trigonal / Hexagonal
E. Cubic
Symmetry Operations

A symmetry operation is a transposition (rotation, inversion, or translation) of an object that leaves the object invariant (unchanged).

- Rotations
  - 360°, 180°, 120°, 90°, 60°
- Inversions (Roto-Inversions)
  - 360°, 180°, 120°, 90°, 60°
- Translations:
  - Unit cell axes and fraction thereof.
- Combinations of the above.

Rotations: may exist in 2 or 3 dimensions

- 1-fold 360°  I  Identity
- 2-fold 180°  2
- 3-fold 120°  3
- 4-fold 90°  4
- 6-fold 60°  6

1-fold Rotation

- 1-fold 360°  I  Identity

Any object has this symmetry

2-fold Rotation

- 2-fold 180°  2
3-fold Rotation
- 3-fold 120°

4-fold Rotation
- 4-fold 90°

6-fold Rotation
- 6-fold 60°

Roto-Inversions (Improper Rotations) three dimensions
- 1-fold 360°
- 2-fold 180°
- 3-fold 120°
- 4-fold 90°
- 6-fold 60°

Roto-Inversions 1-fold
- 1-fold 360°
- Order = 2

Roto-Inversions 2-fold = mirror
- 2-fold 180°
- Order = 2
Stereographic Projections

- We will use stereographic projections to plot the perpendicular to a general face and its symmetry equivalents (general form hkl).
- Illustrated above are the stereographic projections for Triclinic point groups 1 and -1.

Roto-Inversions: 3-fold

- 3-fold 120° followed by inversion
- Order = 6

Roto-Inversions: 4-fold

- 4-fold 90° followed by inversion

Roto-Inversions: 6-fold = 3/m

- 6-fold 60° followed by inversion
- Order = 6

Groups

- A set of elements form a group if the following properties hold:
  - Closure: Combining any two elements gives a third element
  - Association: For any three elements: (ab)c = a(bc)
  - Identity: There is an element, I, such that Ia = aI = a
  - Inverses: For each element, a, there is another element, b, such that ab = l = ba