Symmetry, Groups and Crystal Structures

The Seven Crystal Systems

Minerals structures are described in terms of the unit cell

The Unit Cell

- The unit cell of a mineral is the smallest divisible unit of mineral that possesses 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 interaxial angles (α, β, and γ)

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)

Seven Crystal Systems

- Triclinic \( a \neq b \neq c; \alpha \neq \beta \neq \gamma \neq 90^\circ \neq 120^\circ \)
- Monoclinic \( a \neq b \neq c; \alpha = \gamma = 90^\circ; \beta \neq 90^\circ \neq 120^\circ \)
- Orthorhombic \( a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ \)
- Tetragonal \( a = b \neq c; \alpha = \beta = \gamma = 90^\circ \)
- Trigonal \( a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ \)
- Hexagonal \( a = b \neq c; \alpha = \beta = 90^\circ; \gamma = 120^\circ \)
- Cubic \( a = b = c; \alpha = \beta = \gamma = 90^\circ \)
### Symmetry Operations

A symmetry operation is a transposition of an object that leaves the object invariant.
- **Rotations**
  - 360º, 180º, 120º, 90º, 60º
- **Inversions (Roto-Inversions)**
  - 360º, 180º, 120º, 90º, 60º
- **Translations**
  - Unit cell axes and fraction thereof.
  - Combinations of the above.

### Rotations

<table>
<thead>
<tr>
<th>Order</th>
<th>Rotation</th>
<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-fold</td>
<td>360º</td>
<td>I (Identity)</td>
</tr>
<tr>
<td>2-fold</td>
<td>180º</td>
<td>2</td>
</tr>
<tr>
<td>3-fold</td>
<td>120º</td>
<td>3</td>
</tr>
<tr>
<td>4-fold</td>
<td>90º</td>
<td>4</td>
</tr>
<tr>
<td>6-fold</td>
<td>60º</td>
<td>6</td>
</tr>
</tbody>
</table>

### Roto-Inversions (Improper Rotations)

<table>
<thead>
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<th>Symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-fold</td>
<td>360º</td>
<td></td>
</tr>
<tr>
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<td>180º</td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
<tr>
<td>4-fold</td>
<td>90º</td>
<td></td>
</tr>
<tr>
<td>6-fold</td>
<td>60º</td>
<td></td>
</tr>
</tbody>
</table>

### Translations

- Unit Cell Vectors
- Fractions of unit cell vectors
  - (1/2, 1/3, 1/4, 1/6)
- Vector Combinations

### 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 \(ab = I = ba\).

### 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.
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)

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

Miller Indices

- Plane cuts axes at intercepts (∞,3,2).
- To get Miller indices, invert and clear fractions.
  - (1/∞, 1/3, 1/2) (x6)=
  - (0, 2, 3)
  - General face is (h,k,l)

Miller Indices

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

Stereographic Projections

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

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.