Mineralogy and Petrology: Crystallography

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**Earth Dynamics:**

*Unit cell:* smallest unit of a crystal lattice

*Miller index:* labelling crystal faces

*Symmetry elements:* diad †, triad ▲, tetrad ▼, mirror planes |

*Seven crystal systems* (triclinic-…-cubic)

*Bravais lattices:* Primitive cubic lattice \((a=b=c, \alpha=\beta=\gamma=90^\circ)\)

*Steno’s law:* Constancy of interfacial angles
Crystallography: “The experimental science of determining the arrangement of atoms in a solid.”

Crystal: “A solid with a regular, ordered, repeating pattern extending in all three spatial directions.”

The basic building block or “Unit Cell”
Abbé René-Just Haüy (1743-1826)

Crystals can be constructed by stacking together tiny identical building units (*unit cells*).

Explains ‘Steno’s Law’: law of constancy of interfacial angles (angle between corresponding pairs of faces are constant from one example of a particular mineral species to another).

There are a limited number of ways of stacking unit cells in 3 dimensions.
The seven crystal systems

- All crystals can be described by 7 crystallographic systems

- These systems represent different ways of stacking unit cells of different shapes (see lecture 2)

- Systems are all characterised by:
  - 3 axes (x, y, z)
  - angles between the axes (α, β, γ)
  - relative lengths of the axes (a, b, c)

One system is the exception!
The seven crystal systems

- **Triclinic**
  - $a \neq b \neq c$
  - $\alpha \neq 90^\circ$
  - $\beta \neq 90^\circ$
  - $\gamma \neq 90^\circ$

- **Monoclinic**
  - $a \neq b \neq c$
  - $\alpha \neq 90^\circ$
  - $\beta = 90^\circ$
  - $\gamma = 90^\circ$

- **Orthorhombic**
  - $a \neq b \neq c$
  - $\alpha = 90^\circ$
  - $\beta = 90^\circ$
  - $\gamma = 90^\circ$

- **Tetragonal**
  - $a = a \neq c$
  - $\alpha = 90^\circ$
  - $\beta = 90^\circ$
  - $\gamma = 90^\circ$

- **Hexagonal**
  - $a = a \neq c$
  - $a^\wedge a = 120^\circ$
  - $a^\wedge c = 90^\circ$

- **Trigonal**
  - $a = a = a$
  - $\alpha \neq 90^\circ$
  - $\beta \neq 90^\circ$
  - $\gamma \neq 90^\circ$

- **Cubic**
  - $a = a = a$
  - $\alpha = 90^\circ$
  - $\beta = 90^\circ$
  - $\gamma = 90^\circ$
Labelling crystal faces: the Miller index system

• Widely used system of indexing crystal faces

• Also used (in slightly modified form) to index lattice planes and directions

• The orientation of a crystal surface (or lattice plane), or any surface parallel to it is defined by considering how it intersects the main crystallographic axes

• A simple example….indexing the faces of a cuboid
Labelling crystal faces: the Miller index system

Intersects x axis at a
Intersects y axis at $\infty$
Intersects z axis at $\infty$

Index only needs to give *relative* slope
(i.e. intercept as a proportion of repeat distance).

An index of $(a/a, \infty/b, \infty/c)$ is too clumsy!
Instead, use reciprocals.....

Index is $(a/a, b/\infty, c/\infty)$ or (100)
Labelling crystal faces: the Miller index system

Intersects x axis at $\infty$
Intersects y axis at $\infty$
Intersects z axis at c

Index is $(a/\infty, b/\infty, c/c)$ or $(001)$

(010)
Labelling crystal faces: the Miller index system

Index is \((a/a, b/b, c/c)\) or \((111)\)

Index is \((a/a, b/\frac{1}{2}b, c/\infty)\) or \((120)\)
Plane parallel to (120) but which cuts -x axis and -y axis

Index is \((a/-a, b/-\frac{1}{2}b, c/\infty)\)

or \((\bar{1}20)\)
Miller Indices: general rules

• Miller indices of crystal faces have the general form \((hkl)\)

• A crystal face with an index \((hkl)\) is parallel to a plane that makes intercepts of \(a/h\), \(b/k\) and \(c/l\) on the \(x\), \(y\) and \(z\) axes (where \(a\), \(b\) and \(c\) are unit repeats).

• The face \((111)\) is defined as the ‘parametral plane’, and by definition, intercepts all axes at one unit repeat.

  • when indexing a crystal, the first step is to choose the axes and then pick a parametral plane.

• **Law of rational intercepts:** intercepts of all faces on crystallographic axes are simple fractions or multiples of the intercepts made by the parametral plane.

  • this implies that Miller indices are always whole numbers or zero.

• Miller indices are always simplified to the smallest possible values. Thus, \((486)\) becomes \((243)\). This is because Miller symbols are only concerned with relative slopes.
Miller Indices: labelling crystal faces

- orthorhombic crystal
- Choose 3 mutually perpendicular axes
- Choose a parametral plane (define unit repeats)
Miller Indices: labelling crystal faces

- orthorhombic crystal
- Choose 3 mutually perpendicular axes
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Define as (111)
Miller Indices: labelling crystal faces

• orthorhombic crystal

• Choose 3 mutually perpendicular axes

• Choose a parametral plane (define unit repeats)
Miller Indices: labelling crystal faces

- orthorhombic crystal
- Choose 3 mutually perpendicular axes
- Choose a parametral plane (define unit repeats)

- Second set of faces have intercepts at 2a, 2b and 2/3c
- This can be simplified to 1a, 2b, 1/3c
- Index is, therefore, (113)
Miller Indices: labelling crystal faces

- orthorhombic crystal
- Choose 3 mutually perpendicular axes
- Choose a parametral plane (define unit repeats)

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- This can be simplified to 1a, 2b, 1/3c
- Index is, therefore, (113)
Crystal form

- From the previous slide it is obvious that certain crystallographic faces are related

**FORM:** “a set of symmetrically equivalent faces”

2 forms: {111} and {113}

1 form: {100}
Zones and zone axes

- A ZONE is a set of faces with mutually perpendicular edges.

- The zone with the most conspicuous set of faces is called the ‘prism zone’.

- The common edge direction of these faces is known as a ZONE AXIS.

- Zone axes are labelled [uvw].

Face normals for a zone always lie in a single plane. This plane is at right angles to the zone axis.
Exercise: Consider a tetragonal crystal \(a=b\neq c\). Given the information that the angle between (101) and (001) is 70°, calculate the axial ratio between c and a.

Face (101) is parallel to b (cuts only c and a). Angle between (001) and (101) is 70°, so \(\rho\) is 70°.

\[
\tan \rho = \frac{1c}{1a}
\]

\[
\tan 70 = 2.7475, \text{ so axial ratio for this crystal is } 1:1:2.7475
\]
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Imagine a small crystal at the centre of a vast sphere.
Face poles are projected onto the equitorial plane (primitive circle)
• Now project all points (in upper hemisphere) onto the equatorial plane

• This is done by drawing lines from all points in the upper hemisphere to the south pole
Stereographic projection 3

Lines represent great circles

N.B. face normals for a zone always lie in a plane
Stereographic projection 3

Lines represent great circles

N.B. face normals for a zone always lie in a plane

Northern hemisphere (or +)
Southern hemisphere
Stereographic projection 4: the Wulff net

- Equal angle projection
- Bold lines are 10° divisions
- Faint lines are 2° divisions

- Planes through sphere (i.e. great circles) project as curved lines
- Zones of faces all lie on the same great circle
Stereographic projection 4: the Wulff net

- Equal angle projection
- Bold lines are 10° divisions
- Faint lines are 2° divisions

Small circles are lines of equal angle

Practical 1: use of stereographic projection
Sketch stereograms

Cube

Octahedron

Useful for showing symmetry operators….
Symmetry elements 1: mirror planes

Imagine slicing an object along a plane so that the two halves are exact reflections or mirror images of each other.

Orthorhombic crystal
Symmetry elements 2: inversion and centres of symmetry

A centre of symmetry exists in a crystal if an imaginary line can be extended from any point on its surface, through its centre, to an identical point present along the line equidistant from the centre.

Crystals are described as centrosymmetric or non-centrosymmetric.

Sketch stereogram

N.B. fill dots in N hemisphere
Open symbols in S hemisphere
Symmetry elements 3: axes of rotation

An imaginary line through a crystal about which it may be rotated and repeat itself in appearance.
Symmetry elements 3: axes of rotation

Rotational axes: rotation angle $\alpha$, number of rotations needed to reach origin ($n$)

- $n=2$ $\alpha=180^\circ$
- $n=3$ $\alpha=120^\circ$
- $n=4$ $\alpha=90^\circ$
- $n=6$ $\alpha=60^\circ$