Part 2-1: Crystal morphology

2.1.1 Morphology and Crystal Structure
2.1.2 Law of constancy of the angle
2.1.3 Stereographic Projection
2.1.4 Wulff net
2.1.5 Goniometer
Crystal structure and Morphology

Morphology: the set of faces and edges which enclose a crystal

a) Every crystal face lies parallel to a set of lattice planes; parallel crystal faces correspond to the same set of planes; (hkl)

b) Every crystal edge is parallel to a set of lattice lines.
Crystal growth - Law of constancy of the angle

Crystals of different shapes can result from the same nucleus. But:

In different sample of the same crystal, the angles between corresponding faces will be equal. \textit{(Nicolaus Steno 1669)}

Nucleation $\rightarrow$ growth of a nucleus to a crystal
single crystal $\rightarrow$ morphology
**Stereographic Projection - 1**

**Principle:** Represent **lattice direction** and **plane normal** as point in the projection plane.

**Winkeltreue:** easy measurement of angle in one plane

**Application:** Crystal orientation, Morphology, Symmetry

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p on equatorial plane is the stereographic projection of the pole P on the sphere.

stereographic projection of a **crystal morphology**
Stereographic projection - Example galena (PbS)

Great circles as zone
Stereography - great circle, angle between faces

1. **great circle**: with radius of the sphere;

2. Those faces whose poles lie on a single great circle belong to a **single zone**;

3. The **zone axis** lie perpendicular to the plane of the great circle.

Poles of the faces

The **angle between two poles** means the angle between the **normals n** in a **great circle**.
The angles between crystal faces may be measured with a reflecting goniometer.
Wulff Net - 1

Principle: The Wulff net is the projection of grid net of a globe with North-South-axis (N-S) in the projection plane.

Element: great- und small- circle, equator, pole, azimuth, pole distance
Wulff Net - Angle between faces

Steps:

1. The angle between two faces is the angle between their normals.

2. The two normals define the plane of a great circle.

3. The arc of the great circle between the two normals is the measured angular value.

Angles are measured only from great circles.
The faces of the tetragonal pyramid have \( \varphi \)-coordinates of 0°, 90°, 180° and 270° respectively;

All faces have the same \( \rho \)-value.
Angle between two poles

**Rotate** two poles lie in a great circle:

1. cover the stereogram with Wulff net with the same circle center

2. Rotate the stereogram using the circle center.

Red poles → blue poles
Wulff Net - Application 2

Zone defined by two faces

Case 1: **draw zone pole** corresponding to a zone circle:

1. Rotate the zone circle onto a great circle;
2. Zone pole is 90° from the zone circle along the equator.

Case 2: **draw zone circle** corresponding to a given zone pole

1. Rotate the pole onto the equator;
2. The zone circle is the meridian 90° away from the pole
Known lattice parameters, and consider only faces with low Miller indices

1. Six faces $<100>$
2. From (001), find (101) by $\delta$ and $\delta'$
3. Find other symmetric faces of $<110>$
4. Find (111) by interaction of $[(100)/(011)]$ and $[(101)/(010)]$
Summary - Stereographic projection

1. The angle between faces.

2. Index the crystal zone in stereogram.

3. Great circle
**Gnomonic Projection**

**Prinzip:**
- Mittelpunkt des Kristalls bzw. der Polkugel als Projektionszentrum
- Projektion auf die Tangentialebene durch den Nordpol
Part 2-2: Principles of Symmetry

2.2.1 Rotation axes

2.2.2 The mirror plane

2.2.3 The inversion center

2.2.4 Compound Symmetry operations

2.2.5 Rotoinversion axes

2.2.6 Rotoreflection axes
Allen Gittern gemeinsam ist die Translationssymmetrie. (Einwirkung von 3 nicht komplanaren Gitter-Translationen auf einen Punkt ⇒ Raumgitter)

Andere Symmetrieigenschaften treten nicht notwendigerweise in jedem Gitter auf.

Die Translationssymmetrie schränkt die Zahl denkbarer Symmetrieelemente drastisch ein.
Symmetry - Basic conceptions

All repetition operations, lattice translations, rotations and reflections, are called symmetry operations.

When a symmetry operation has a “locus”, that is a point, a line or a plane that is left unchanged by the operation, this locus is referred to as the symmetry element.

Symmetry element:
- Mirror plane
- Rotation axis
- Inversion center
The symmetry element corresponding to the symmetry operation of rotation is called a rotation axis.

The order of the axis is given by $X$ where $X=360°/\varepsilon$ and $\varepsilon$ is the minimum rotation angle.

Objects are said to be equivalent to one another if they can be brought into coincidence by a symmetry operation.
Rotation axes - 2

Three-fold rotation axis: $3(\Delta)$

- 120°

Fourth-fold rotation axis: $4(\Box)$

- 90°

Six-fold rotation axis: $6(\bigcirc)$

- 60°
No 5- or 7-fold rotation

Five-fold rotation does not constitute a lattice plane.

Rotation axes order **higher than 6** do not constitute a lattice plane.

Parallele Gittergeraden müssen gleiche Translationsperiode haben.
<table>
<thead>
<tr>
<th>Rotation angle</th>
<th>Symbol</th>
<th>Graphic Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>360°</td>
<td>1 (nach Hermann-Mauguin)</td>
<td>-</td>
</tr>
<tr>
<td>180°</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>120°</td>
<td>3</td>
<td>△</td>
</tr>
<tr>
<td>90°</td>
<td>4</td>
<td>◊</td>
</tr>
<tr>
<td>60°</td>
<td>6</td>
<td>◦</td>
</tr>
</tbody>
</table>
Mirror Plane

The symmetry element of reflection is called mirror plane or plane of symmetry symbol is: \( m \)

Any point or object on one side of a mirror plane is matched by the generation of an equivalent point or object on the other side at the same distance from the plane along a line normal to it.
Inversion Center

The symmetry operation, inversion, relates pairs of points or objects which are equidistance from and on opposite sides of a central point. The symbol is: 1

Inversion at 1/2, 1/2, 1/2.

Each space lattice has inversion operation; All lattices are centrosymmetric.
**Compound symmetry operations**

**Compound symmetry operation**
Two symmetry operations are performed in sequence as a single event. This produces a new symmetry operation but the individual operations of which it is composed are lost.

*Example:* Rotation of 90° about an axis followed by an inversion through a point on the axis.

**Combination of symmetry operation**
Two or more symmetry operations are combined which are themselves symmetry operations.

*Example:* 4-fold rotation and inversion
The compound symmetry operation of rotation and inversion is called *rotoinversion*. Its symmetry elements are the *rotoinversion axes*, general symbol: $\bar{X}$

Note:
Only rotoinversion axes of odd order imply the presence of an inversion center, $\bar{1}$ and $\bar{3}$. 
Compound symmetry - Rotoreflection axes

*Rotoreflection* implies the compound operation of *rotation and reflection* in a plane normal to the axis.

\[ S_1 \equiv m; \quad S_2 \equiv 1; \quad S_3 \equiv \bar{6}; \quad S_4 \equiv \bar{4}; \quad S_6 \equiv \bar{3}. \]

**Symmetry elements:**

- **proper rotation axes** \( X(1, 2, 3, 4 \text{ and } 6) \) and
- **rotoinversion** or improper axes \( \bar{X}(1 \equiv \text{inversion center}, \quad 2 \equiv m, \quad 3, 4 \text{ and } 6) \)

The axes *rotation axes* \( X(1, 2, 3, 4 \text{ and } 6) \) and *rotoinversion axes* \( \bar{X}(1 \equiv \text{inversion center}, \quad 2 \equiv m, \quad 3, 4 \text{ and } 6) \), including \( \bar{1} \) and \( m \), are called **point-symmetry elements**, since their operation always leave at least one point unmoved.
Summary - Symmetry basis

Mirror
rotation
inversion

rotoinversion = rotation + inversion
rotoreflection = rotation + mirror