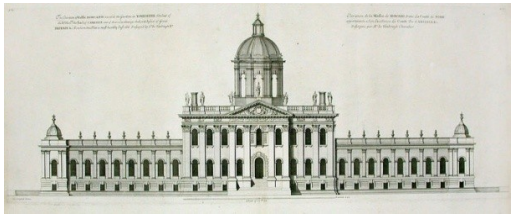
Symmetry:
theoretical concept versus practical meaning

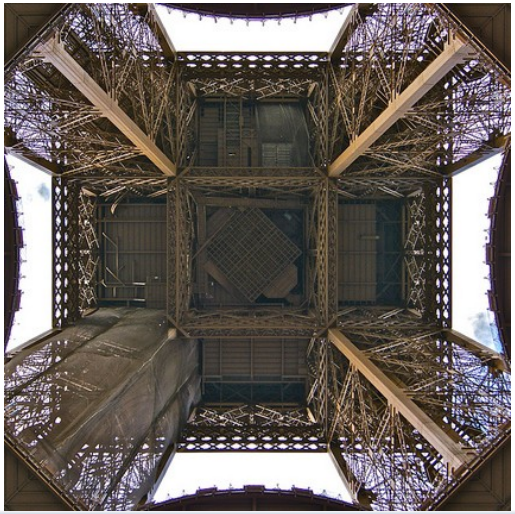
G. Nolze

[1]*Federal Institute for Materials Research and Testing (BAM), Berlin, Germany*

1. Introduction
2. Crystallographic symmetries
3. Pseudo-symmetries
4. Symmetry inheritance
5. Sample and process symmetries

Examples of artificial symmetry





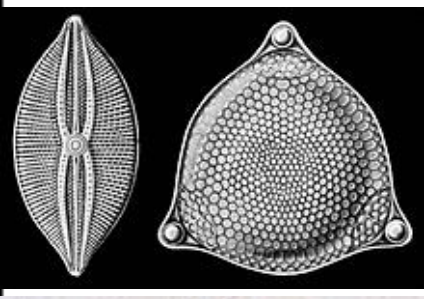
Grammichele (Sicily)

Goryokaku (Japan)

Nature and symmetry

Bundesministerium
für Wirtschaft
und Technologie

BAM



Symmetry is the peak of perfection.

or

Does symmetry only *appears* to be the peak of perfection?

Why do we think so?

…because we are part of the "system" nature.

But: There are many other opinions which think that symmetry is boring, and only chaos or deviation of symmetry is beautiful.

Beauty is in the eye of the beholder.

What is symmetry?

What is and why do we use symmetry?

Bundesministerium für Wirtschaft und Technologie

BAM

Comes from Greek ”συμμετρία” (*symmetria)* and means agreement in dimensions, due proportion, arrangement etc.

- In **everyday language** it refers to a sense of harmonious and **beautiful proportion** and **balance**.
- In **mathematics** (crystallography) symmetry has a more precise definition:

  An object is invariant to transformations!

  (such as rotations, roto-inversions, reflections, …and translations)
- In **practice**, symmetry is the **synonym of** maximum **efficiency** in energy, resources, costs, time, loss-free data compression…

  It is some kind of laziness ☺.
- Therefore, the driving force is huge in order to develop, produce, analyze…in shortest time, with minimum resources, error free etc.

Let’s look for symmetry…in crystals!

Crystallographic symmetry

Which crystallographic symmetries are relevant (for us)?

1. 6 translation lattices (7 **crystal systems**)
   for 4/m and 4/mmm; -3 and -3m; 6/m and 6/mm; or m-3 and m-3m EBSD patterns are often very similar!

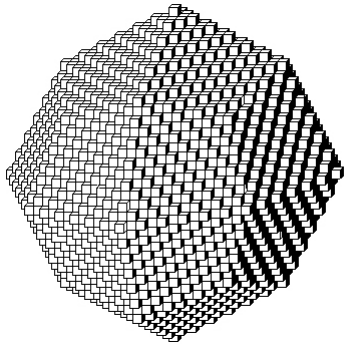
2. 32 **point** symmetry **groups** (crystal classes)
   suitable for the description of physical or chemical properties, e.g. the anisotropic distribution of diffracted intensity in EBSD patterns (!)

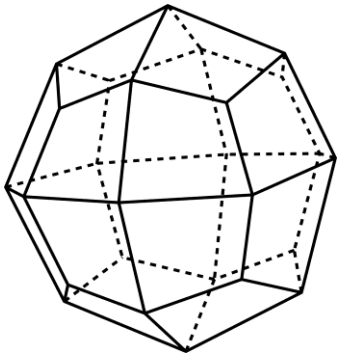
   - 11 centro-symmetric **Laue groups**
     subset of the 32 point groups. Per default they are used to describe diffraction phenomena like EBSD. Used for IPF-colouring.

   - 21 non-centrosymmetric groups:
     ⇨ 11 **enantiomorphic groups** (rotational, chiral,)
     used for unique orientation colouring (fundamental sector)

3. 230 **space-group** symmetry groups
   Generation of unit cell content. Defines the visibility of bands!

Symmetry in crystals



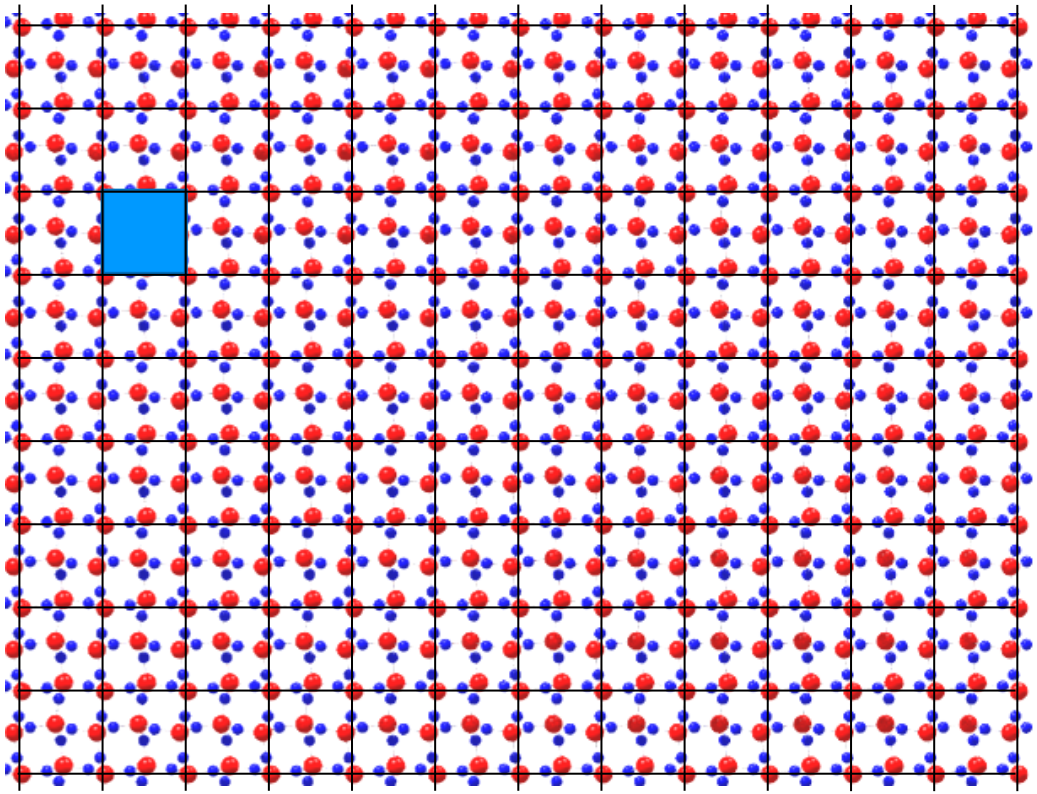


- Crystals are commonly understood as nonliving materials with a high degree of order (symmetry).
- *History:* Cleavage experiments showed that crystals could be an arrangement of tiny and identical polyhedra.

  Now we know: Each polyhedron represents a **point** in an infinitely expanded **lattice** which is mainly defined by its **translation symmetry** (unit cell).
- The **lattice point represents** the content of a (primitive) unit cell which can contain only one but also thousands of atoms and their **space-group symmetry**.
- The habit of regular crystals macroscopically reflects the **point group symmetry**, but also other **physical** and chemical **properties** are point-group related (anisotropy).
- Unfortunately, common **diffraction phenomena** (EBSD?) are assumed to be centrosymmetric which enables the characterization of centrosymmetric **Laue groups** only.

Why symmetries?

The major sense of a crystallographic description is to reduce the data as much as possible.
The easiest kind is the **translation symmetry**.



This is the structure of Crystobalite: SiO_2

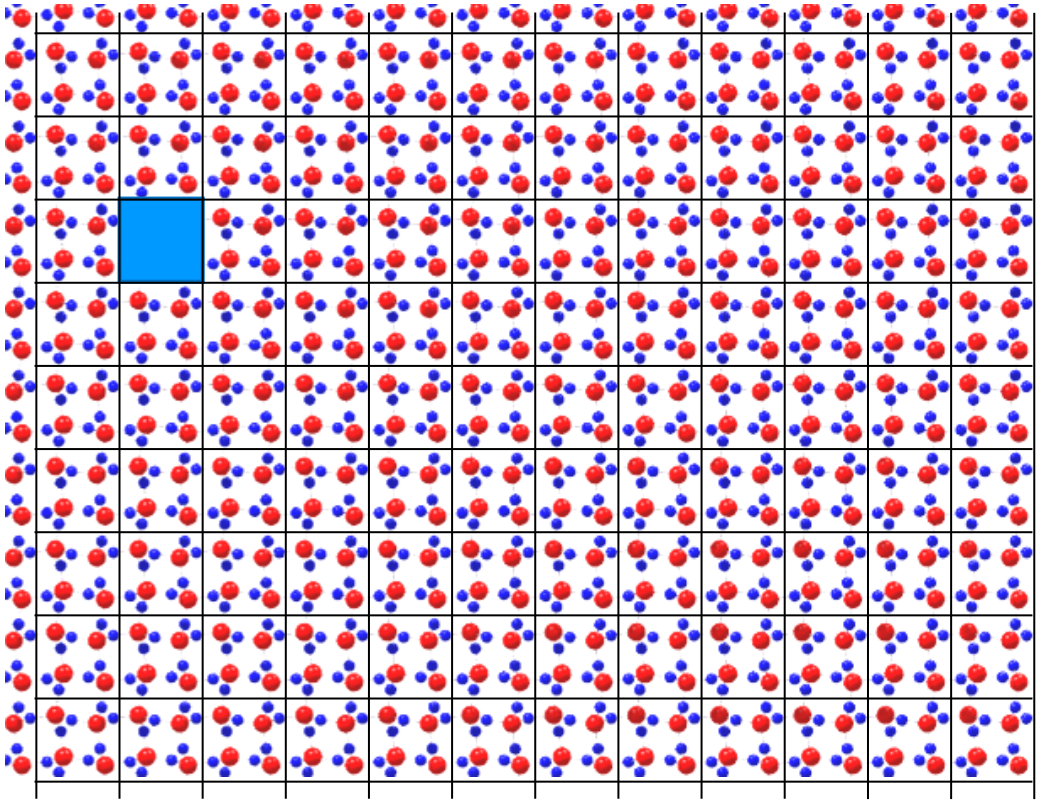
It has obviously some kind of **motif** which appears endlessly after applying a **translation operation**.

Why symmetries?

Bundesministerium für Wirtschaft und Technologie

BAM

The major sense of a crystallographic description is to reduce the data as much as possible.
The easiest kind is the **translation symmetry**.



This is the structure of Crystobalite: SiO_2

It has obviously some kind of **motif** which appears endlessly after applying a **translation operation**.

We can generate the entire structure by application of translations **along three basic vectors**:

$$\vec{R} = u \cdot \vec{a} + v \cdot \vec{b} + w \cdot \vec{c}$$

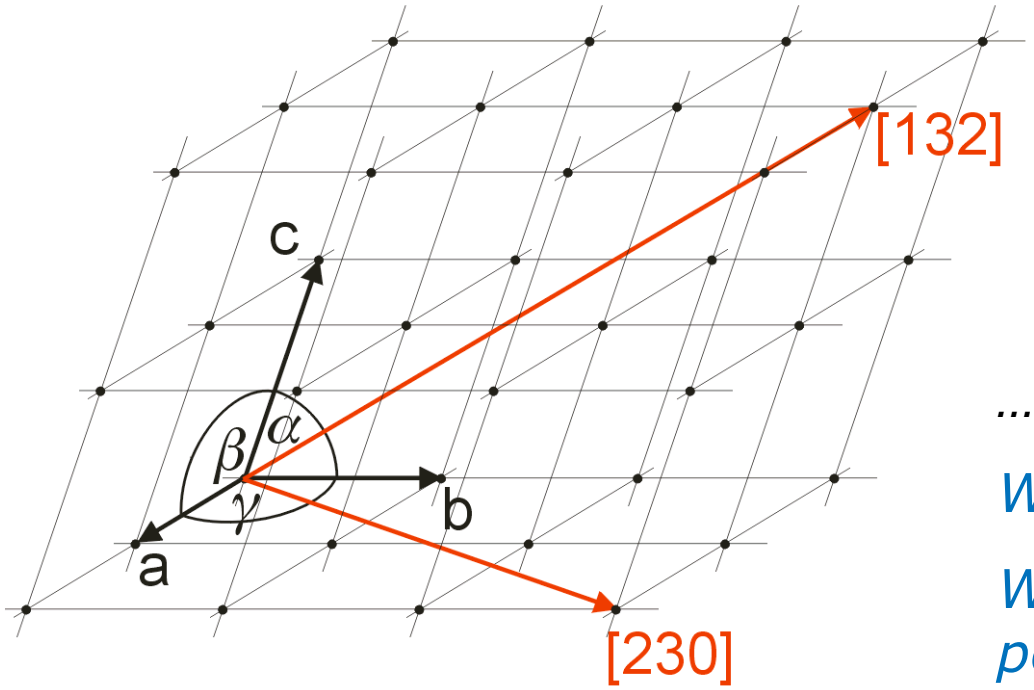
u, v, w are integers

Translation symmetry: crystal lattice

Bundesministerium für Wirtschaft und Technologie

BAM

The lattice is a **mathematical abstraction** of a crystal where the motif is replaced by a lattice point. Since the lattice appears as endless-repeating pattern one needs only the knowledge about the smallest unit. The **unit cell** is defined by three basis vectors of the length **a**, **b**, **c**, and the angles α, β, γ lying in-between.



a, **b**, **c** and α, β, γ are called lattice parameters or simply lattice constants.

They are phase-specific !

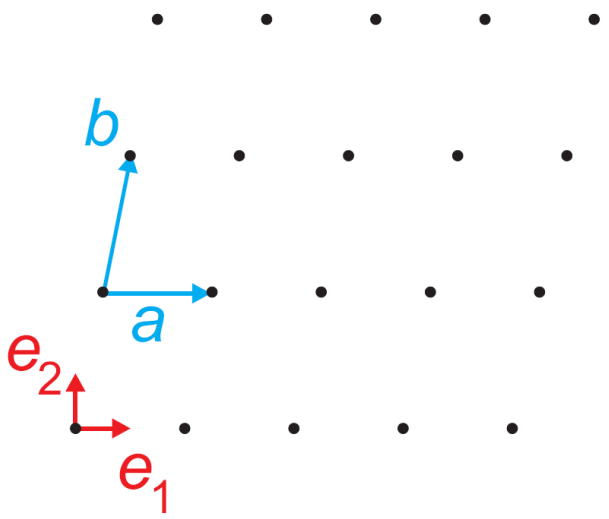
…this should be clear, but…

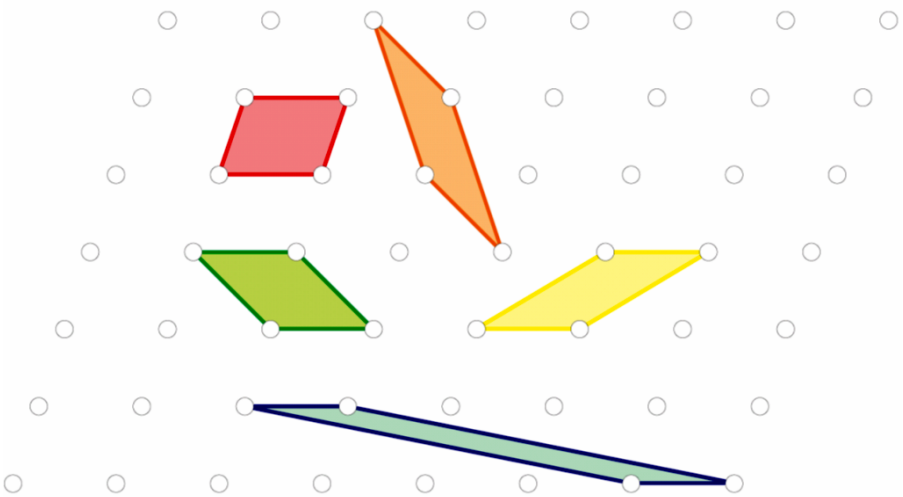
Who defines the basis vectors?

What defines the atomic positions?

The unit cell

The unit cell is defined as smallest volume which enables a complete crystal reconstruction by translations in all three directions only.



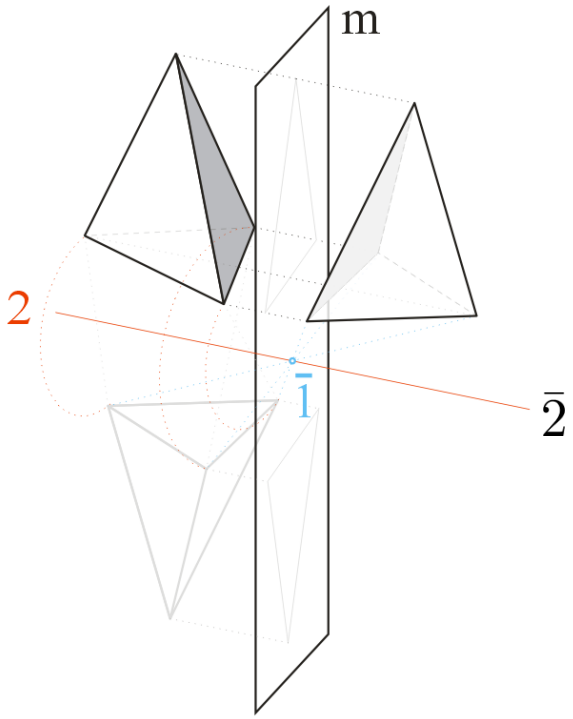


⇨ For the same lattice countless unit cell definitions are imaginable.

Recommended are: - the shortest vectors
- the angle in-between are preferred to be ≥ 90°

But: Is this a really useful definition?

Symmetry elements in point groups



Example of rotation, inversion and roto-inversion with multiplicity 2.

A **translation** t shifts the motif &: 

A **rotations** R moves a motif around an axis. After R rotations the identity is given: 

A **symmetry center** $\bar{1}$ inverts a motif: 

red colored motif expresses the inverted character

A **roto-inversion** is the combination of rotations combined with an inversion: 

It generates half that many original and half that many inverted motifs, i.e. the multiplicity is always an even number, also for $\bar{1}$ *and* $\bar{3}$.

The **mirror plane** is a roto-inversion: 

$$m = \bar{2}$$

All symmetry operators generating red–colored motifs are improper operators. Written as matrix, their determinant is -1.

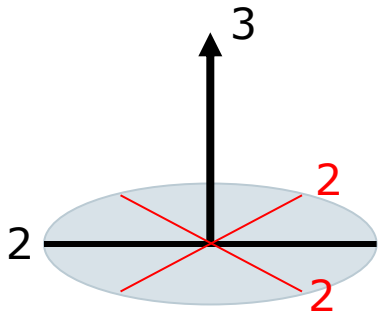
Point group symmetry

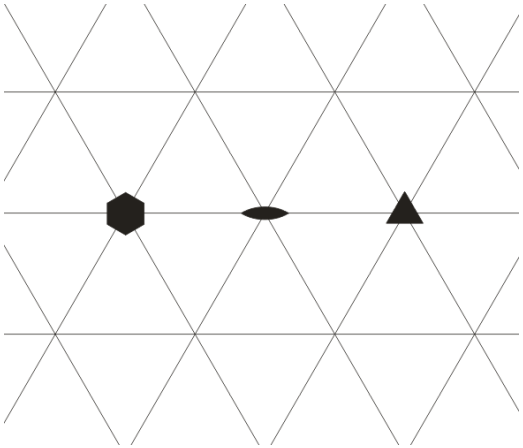
A **point group** is an arrangement of symmetry operators.
It is called point group since it **keeps** at least **one point fixed**.

Please note:

1. A **symmetry** operator is not only **applied** to motifs but also **to all** other **symmetry operators**.
2. Any symmetry operation has to **match** to all symmetry elements, in particular to **the translation symmetry** of the lattice.

⇨ In general, only rotations R with the multiplicity 1, 2, 3, 4 and 6 are permitted.





Point group symmetry

Bundesministerium für Wirtschaft und Technologie

BAM

A **point group** is an arrangement of symmetry operators.
It is called point group since it **keeps** at least **one point fixed**.

Please note:

1. A symmetry operator does not work only on motifs but also on all other symmetry operators.
2. Any symmetry operation has to match to all symmetry elements, in particular the translation symmetry of the lattice.

⇨ In general, only rotations R with the multiplicity 1, 2, 3, 4 and 6 are permitted.

⇨ From this follows: **Only specific angles between symmetry operators** arise as result of the group symmetry, cf. 1.

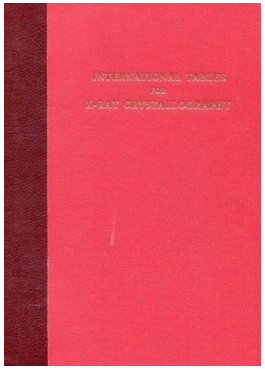
"cubic branch"

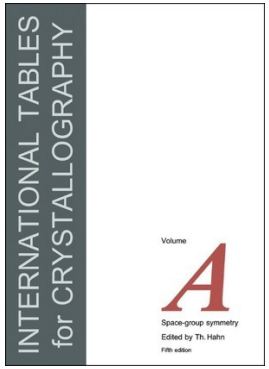
R_1	R_2	∠
4	4	90°
	3	≈ 55°
	2	90°, 45°
3	3	≈ 70°
	2	90°, ≈ 35°
2	2	90°, 60°, 45°

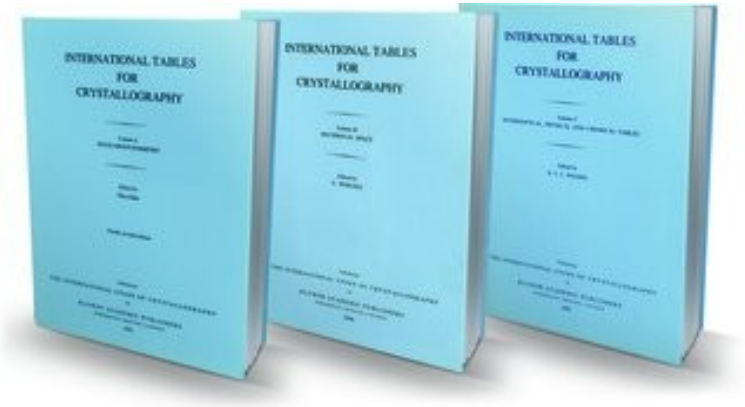
"hexagonal branch"

R_1	R_2	∠
6	2	90°
3	2	90°
2	2	90°, 60°, 30°

International Tables for Crystallography







- The International Tables (IT) for Crystallography represent the **bible** for crystal symmetry description in 2 and 3D.
- It defines applicable regulations in order to make sure that scientists around the world understand each other.
  (like the general use of the metric system)
- IT are under continuous development, i.e. rules can change …and changed over the time (different editions)!
- Vol. A contains **the 230 space groups** which **represent** the internationally accepted, mathematically possible **construction plans** for crystals in 3D.

How they are described?

Directions of symmetry axes

Bundesministerium für Wirtschaft und Technologie

BAM

In order to describe symmetries an international nomenclature has been introduced in 1928 by Carl Hermann, and modified by Charles-Victor Mauguin (1931).

	Position 1.	2.	3.
Triclinic			
Monoclinic (both settings)	[001]	[100]	[010]
Orthorhombic			
Tetragonal	[001]	[100]	[110]
Hexagonal	[001]	[100]	[210]
Rhombohedral	[111]	$[1\bar{1}0]$	$[2\bar{1}\bar{1}]$
Cubic	[001]	[111]	[110]

- The IT- or Hermann-Mauguin symbol defines the direction of **symmetry axes related to** the **basis vectors** of the crystal lattice.
- If the **symmetry directions** are **fixed** by **crystal directions**, the **basis vectors** are **not free definable**, anyway which length these vectors have or which angles are between them.
- Another (often ignored) peculiarity:

$\bar{6}\,m\,2 \qquad 6 \parallel [001] \quad m = \bar{2} \parallel [100] \quad 2 \parallel [210]$

$\bar{6}\,2\,m \qquad 6 \parallel [001] \quad 2 \parallel [100] \quad m = \bar{2} \parallel [210]$

$\bar{4}2m, \bar{4}m2, 321, 312, 31m, 3m1, \bar{3}1m, \bar{3}m1, \bar{6}2m, \bar{6}m2$

Hermann-Mauguin (H-M) symbol

- H-M symbols are given in short and long form: $m\bar{3}m = 4/m\ \bar{3}\ 2/m$
- Mirror planes are defined by their normal directions, i.e. $\| \bar{2}$.
- If symmetry axis and mirror planes are perpendicular to each other (normal parallel to the axis) both letters are separated by a slash, e.g. $P\ 2/m$.
- Directions without any special symmetry are filled by the symbol *1* for identity: e.g. 321 and 312
  They are not necessary if misinterpretations are excluded, e.g. $P\ 6$ instead of $P\ 611$. However, in case of monoclinic space groups the complete H-M symbol enables the differentiation between standard settings – b as monoclinic axis – and non-standard settings – c and a as monoclinic axes.
- For higher-symmetric point groups existing symmetry elements are often omitted, e.g. $P\ mmm$.
  The extended symbol also displays the axes perpendicular to the given mirror planes: $P\ 2/m\ 2/m\ 2/m.$ s
- Please note: There are at least that many symmetry operators as the multiplicity of the group defines.

Derivation of 32 point groups:

Combination of rotations R and $\bar{1}$

Bundesministerium für Wirtschaft und Technologie

BAM

R						
$\bar{R}$						
R/m						
$R2$						
Rm						
$\bar{R}m$						
$R/m\,m$						

Derivation of 32 point groups:

Combination of rotations R and $\bar{1}$

Bundesministerium für Wirtschaft und Technologie

BAM

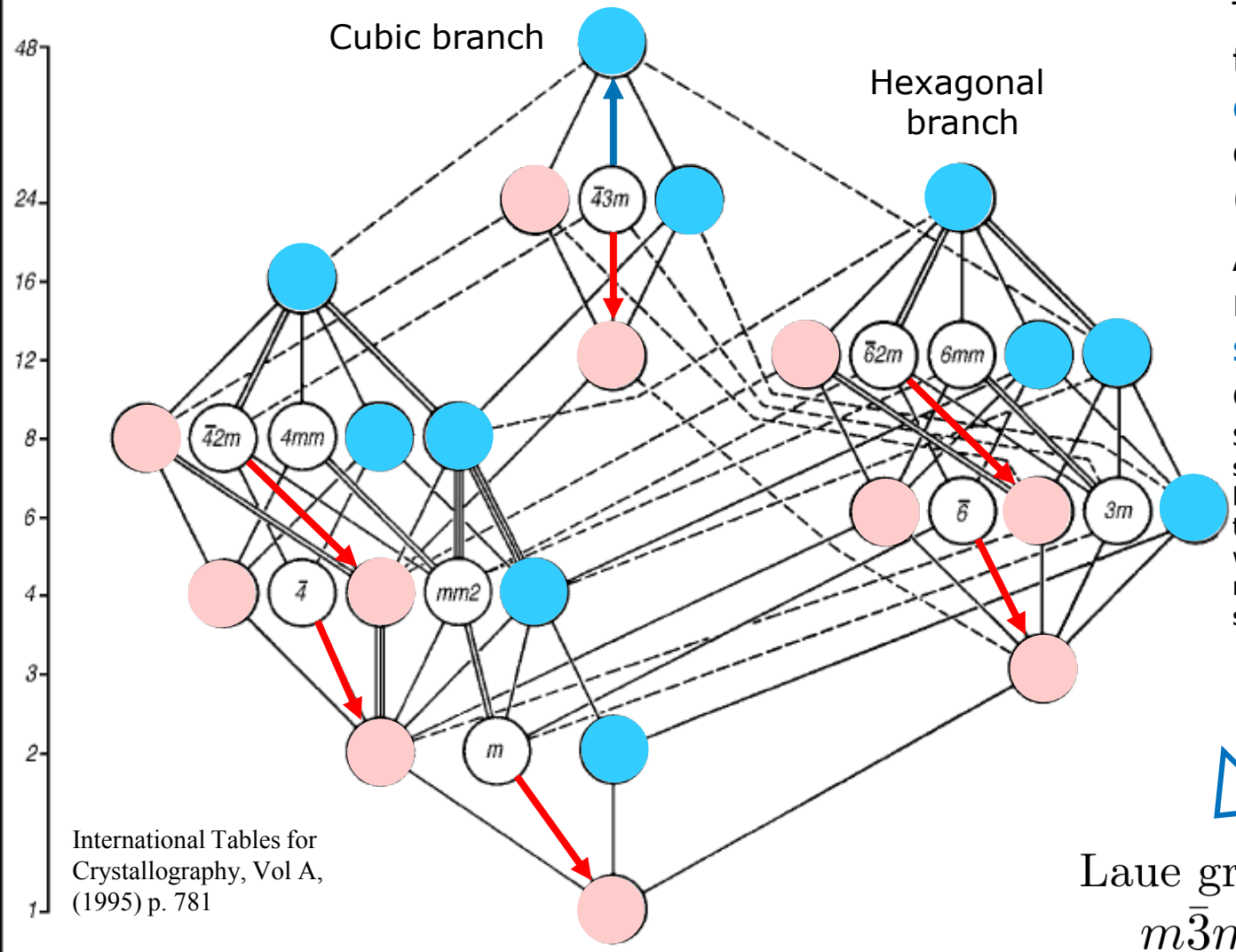
	triclinic	monoclinic/ orthorhombic	trigonal	tetragonal	hexagonal	cubic
R	1 1	2 2	3 3	4 4	6 6	12 23
$\bar{R}$	2 $\bar{1}$	2 [redacted]	6 $\bar{3}$	4 [redacted]	6 $\bar{6}$	$\bar{2}3 = 2/m\bar{3}$
R/m	m	4 $2/m$	$3/m = \bar{6}$	8 $4/m$	12 $6/m$	24 $2/m\,\bar{3}$
$R2$	2	4 222	6 32	8 422	12 622	24 432
Rm	m	4 [redacted]	6 [redacted]	8 [redacted]	12 [redacted]	$2m3 = 2/m\bar{3}$
$\bar{R}m$	$2/m$	$mm2$	12 $\bar{3}m$	8 [redacted]	12 [redacted]	24 [redacted]
$R/m\,m$	$mm2$	8 mmm	$3/m\,m = \bar{6}2m$	16 $4/m\,mm$	24 $6/m\,mm$	48 $m\bar{3}m$

enantiomorphic (chiral) groups

proper rotations

centrosymmetric Laue groups

Subgroup relationships



International Tables for Crystallography, Vol A, (1995) p. 781

This diagram visualizes the derivation of the centrosymmetric (Laue) or enantiomorphic (rotational) groups.

A subgroup always means a reduction, a supergroup an increase of multiplicity.

Solid lines indicate maximal normal subgroups; double or triple solid lines mean that there are two or three maximal normal subgroups with the same symbol. Dashed lines refer to sets of maximal conjugate subgroups.

$\bar{4}3m$

Laue group $m\bar{3}m$

rot. group 23

Example: phase transformation

Bundesministerium für Wirtschaft und Technologie

BAM

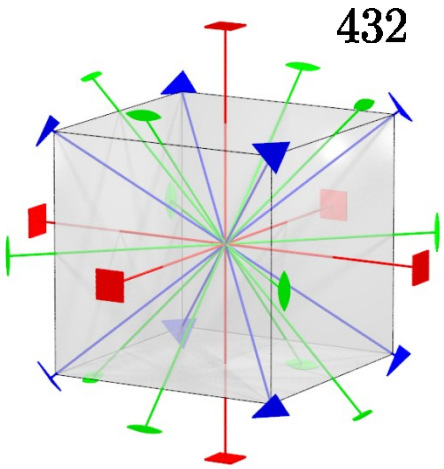
Transformation between different modifications is often a **loss or increase of symmetry**!

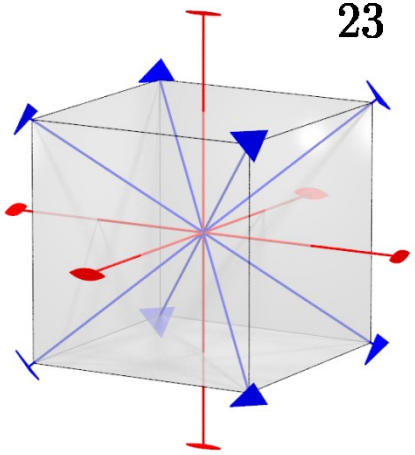
Certain external or internal factors force a material to change the structural arrangement of atoms.

Examples: perovskite (doping),
ZrO_2 (doping),
magnetite-hematite (diffusion),
austenite-ferrite (diffusion, temperature),
Ti-Al
…

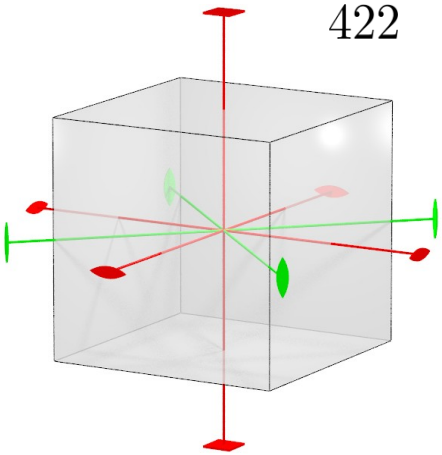
Often only a simple reduction of symmetry is used to increase a degree of freedom.
This is often simply displayed **subgroup relationships**.

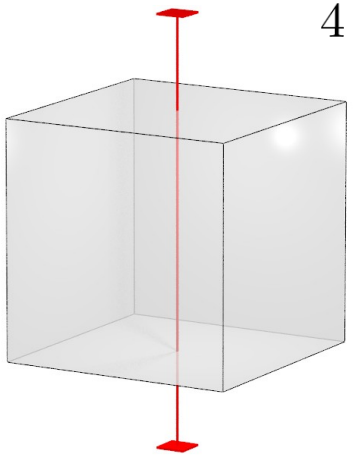
Cubic ⇨ tetragonal





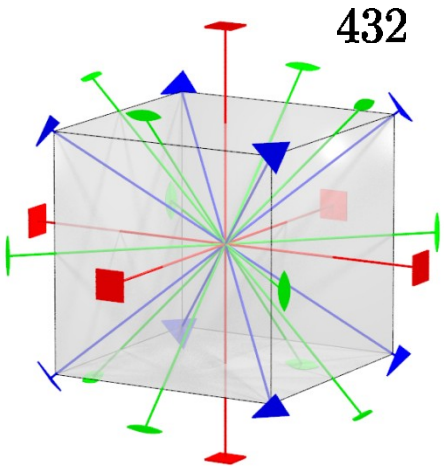
- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.



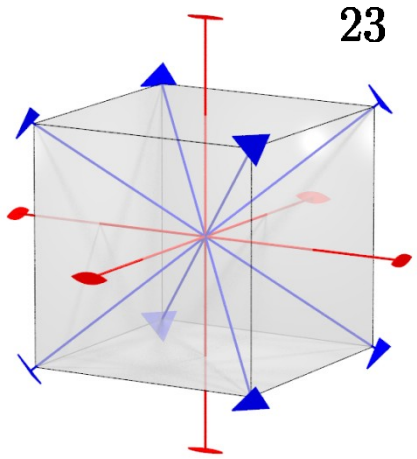


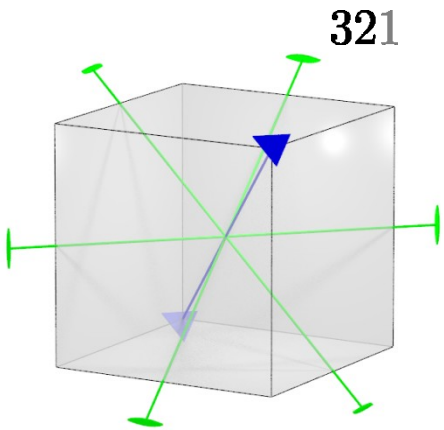
a_3 becomes independent from a_1 and a_2.

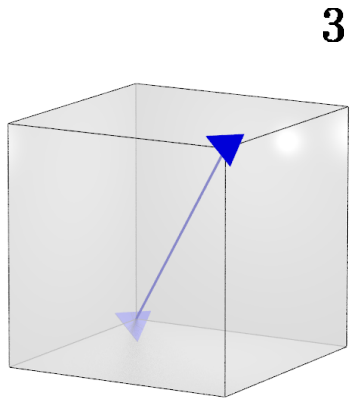
Cubic ⇨ rhombohedral



- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.

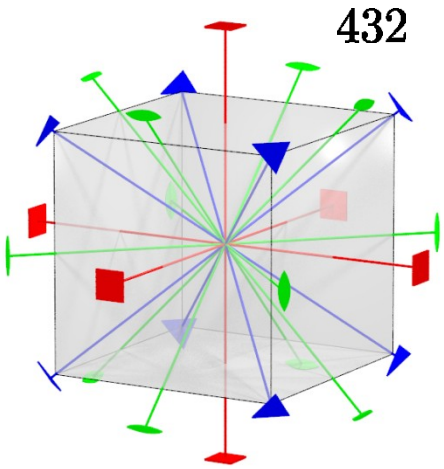




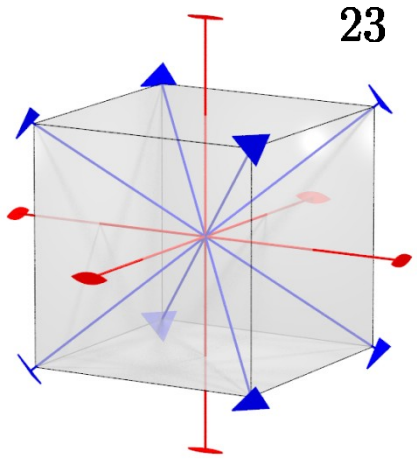


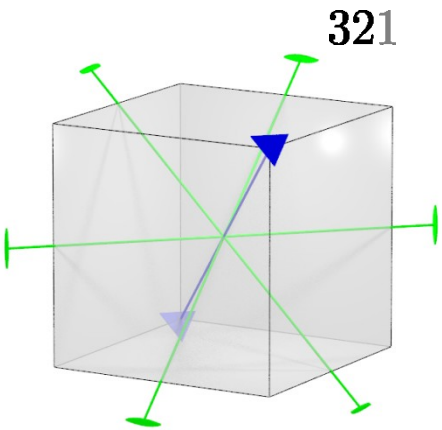
a_1, a_2 and a_3 are identical… but α is free.

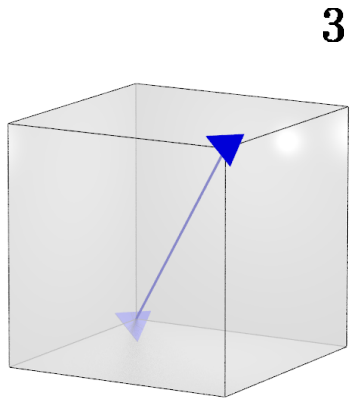
Cubic ⇨ trigonal



- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.

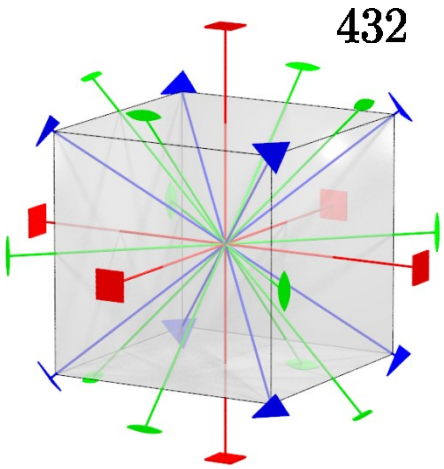




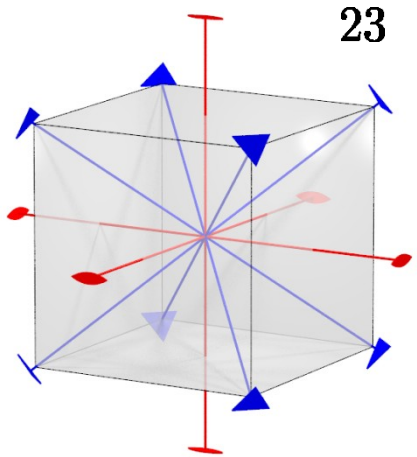


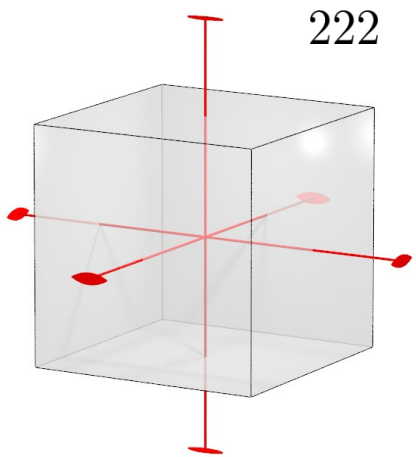
a and c are independent. $\gamma = 120°$

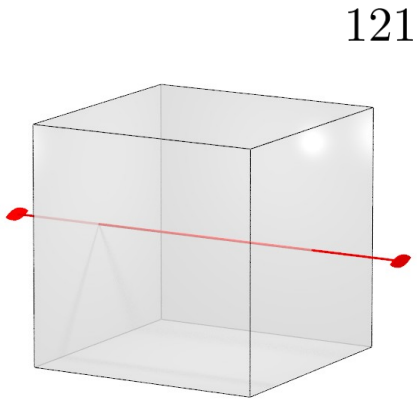
Cubic ⇨ orthorhombic, monoclinic



- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.

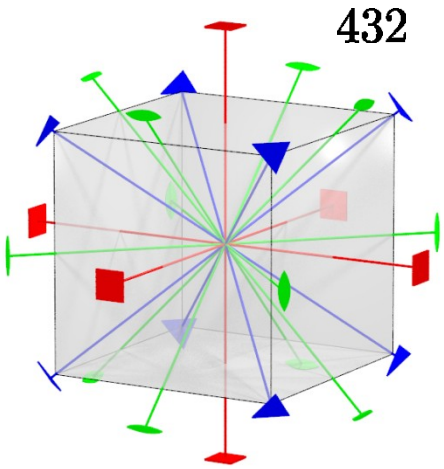




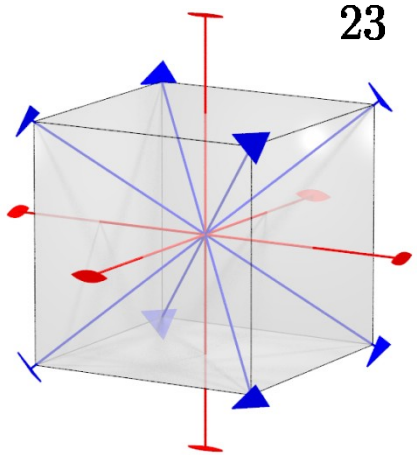


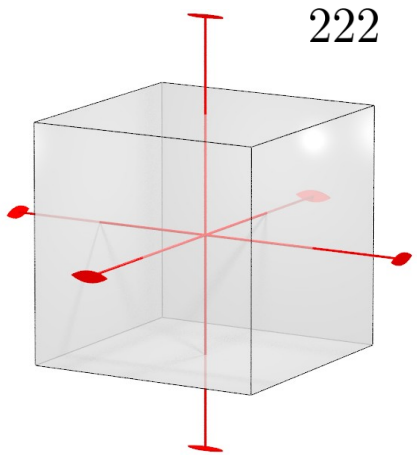
a_1 , a_2 and a_3 are free. β can have any size.

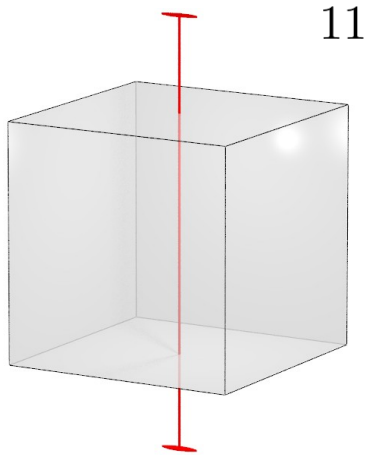
Cubic ⇨ orthorhombic, monoclinic



- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.

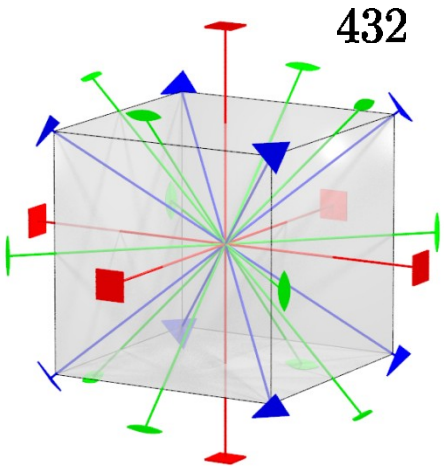


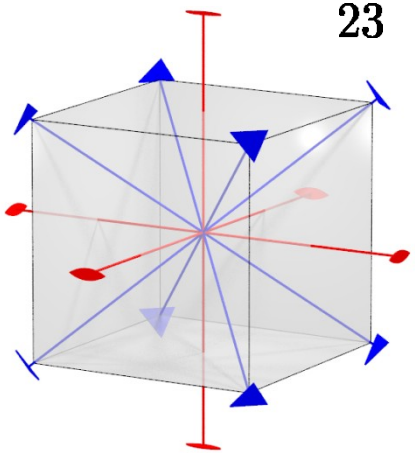




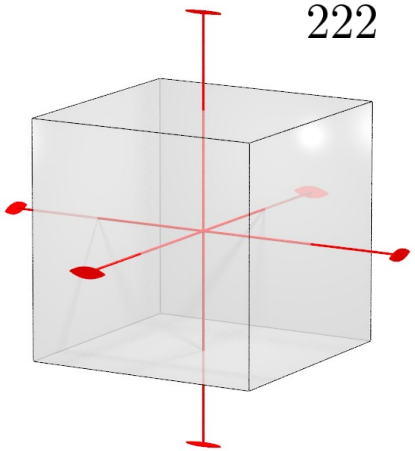
a_1 , a_2 and a_3 are free. γ can have any size.

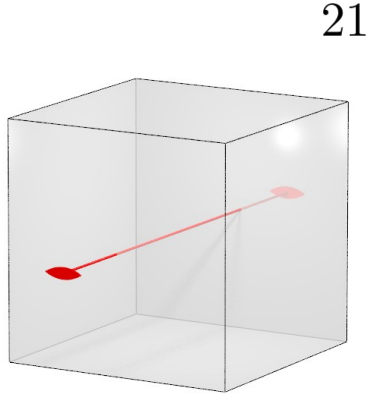
Cubic ⇨ orthorhombic, monoclinic





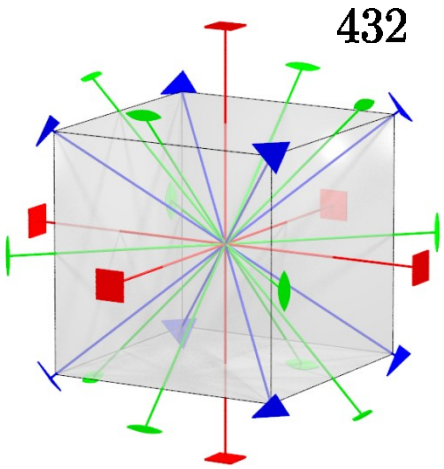
- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.

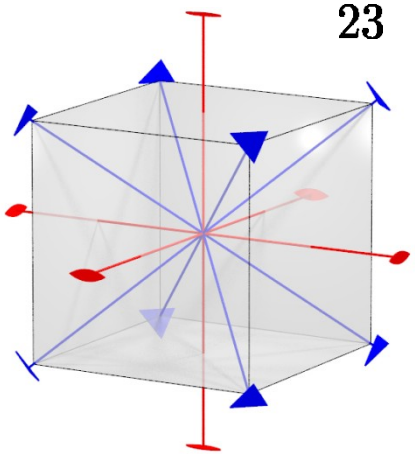




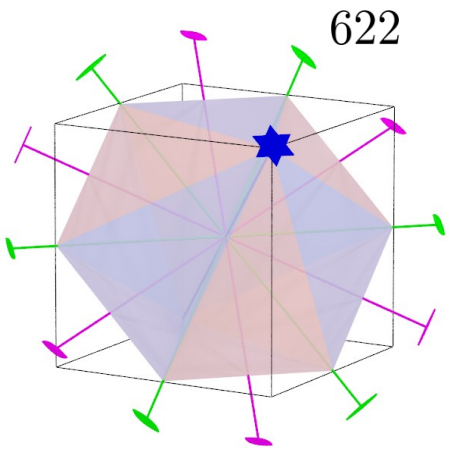
a_1 , a_2 and a_3 are free. α can have any size.

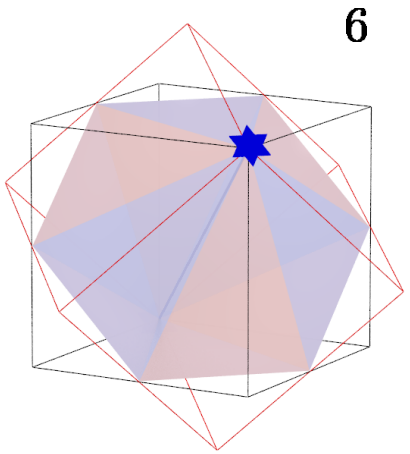
Special case: hexagonal





- The combination of symmetry elements is strongly limited. Here the enantiomorphic groups are shown.
- Starting from highest symmetry and reducing it only groups with less symmetry can be the result.
- Removal of one element often has the consequence, that some other elements disappear as well.





$2 \parallel \langle \bar{2}\,1\,1 \rangle \perp [1\,1\,1] \parallel 3$

First conclusions

- The **symmetry** is the only criterion which **decides about** the definition of **basis vectors**.
  ⇨ *e.g. non-standard settings of space-groups*

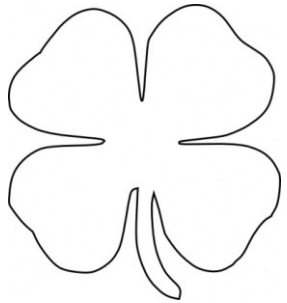
- The **symmetry decides about the crystal system** (cubic, hexagonal etc.) and not the metric of a unit.
  ⇨ *it defines automatically which conditions the unit cell has to fulfill*

- The **angles** between symmetry elements **are constants**.
  ⇨ *for a special symmetry group the symmetry character of any direction is independent of the phase.*

- During **phase transformations** often a simple **symmetry reduction or increase** is observed.
  ⇨ *subgroup or supergroup relationships*

PSEUDO SYMMETRY

Pseudo-symmetry



Is this cloverleaf symmetric or not?

From a mathematical point of view definitely not.

This is exactly the answer in crystallography.

Practically we have to decide, what is possible to distinguish by

- the crystal lattice (6),
- the Laue group (11),
- the point group (32), or even
- the space group (230)?

Crystallographic symmetry only gives the **maximal symmetry**.

thus, the **metric** – i.e. lattice parameters **- can reflect** a clearly **higher symmetry** (hexagonal-orthorhombic phases, martensite, Ti-Al…) properties - e.g. diffraction phenomena – may speak for higher symmetry (Ni-based superalloys)

Lattice symmetry

Bundesministerium für Wirtschaft und Technologie

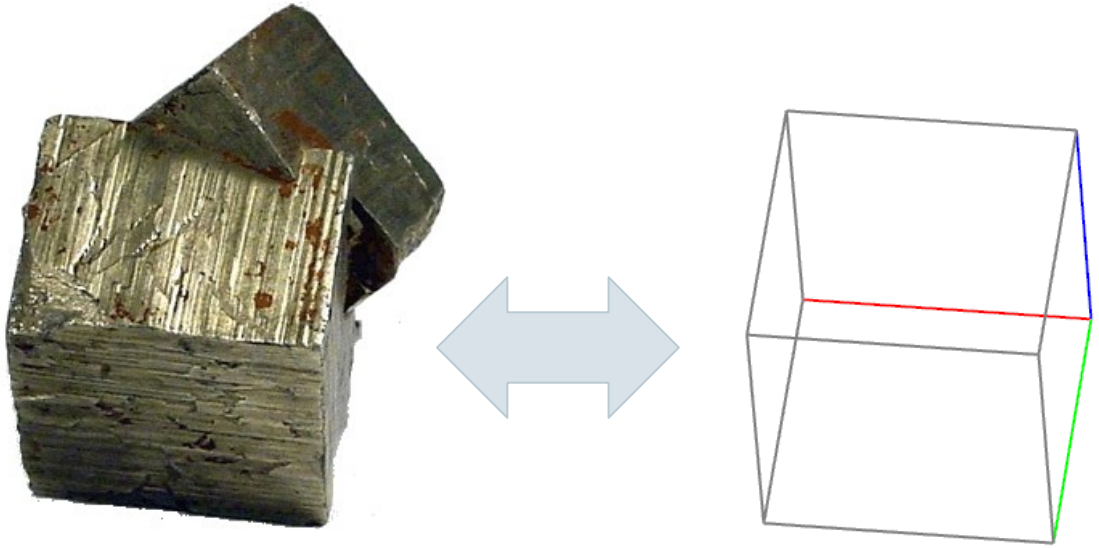
BAM

The lattice symmetry corresponds to the highest point-group symmetry of the respective crystal system. For pyrite (FeS_2) which contains to Laue group m-3, this lower symmetry is often not recognizable (NO 4-fold axes!)

Only sometimes the cube planes display a characteristic striation which points out a missing four-fold rotation symmetry parallel to the cube edges.

It is the maximal symmetry of the polyeder we will be deceived.

EBSD often has no other choice to use the lattice symmetry!



Pseudo-symmetry in Kikuchi patterns

Kikuchi patterns are often only roughly interpreted for certain reasons

- Automatic system, i.e. the real data are often ignored
- Low pattern resolution (small deviations are hard to see)
- General problem: band positions only (no intensity, no band width)
- Pattern formation in general not well understood, models are misinterpreted
- …

However, there is a much more interesting question:

Which differentiation actually makes sense?

The aim of all these investigations is the practical impact of the anisotropy of a certain property!

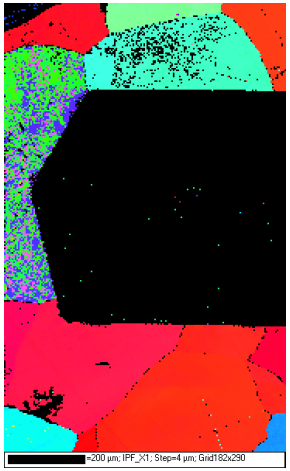
Speckled grains:

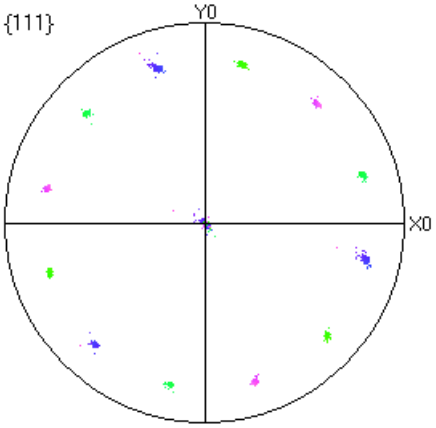
Pseudo-symmetry

Bundesministerium für Wirtschaft und Technologie

BAM

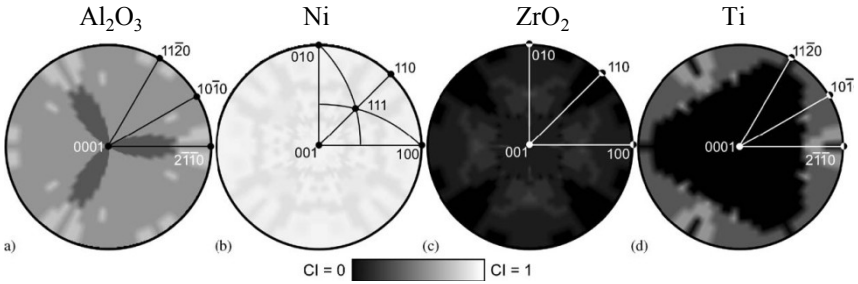
in EBSD patterns





α-Fe, m3m

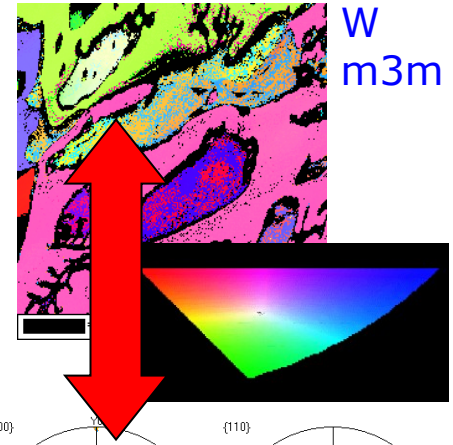
- for specific orientations in patterns a virtually higher symmetry appears

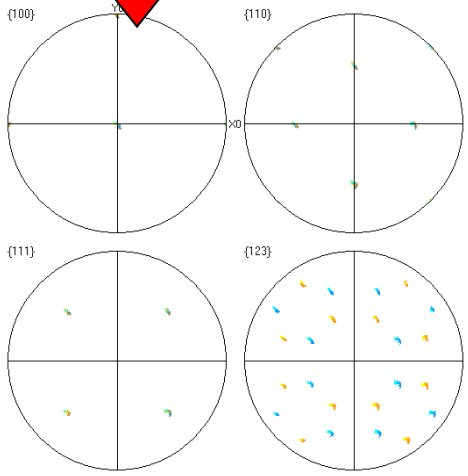


Novell, Wright ,Ultramicroscopy **103** (2005), 41-58

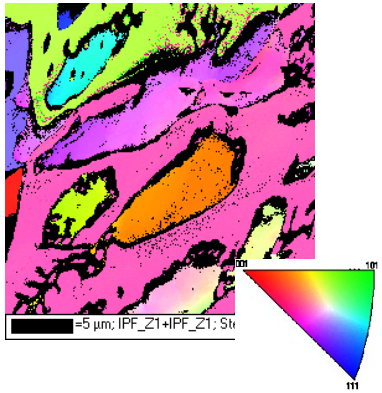
Crystal symmetry

La_2O_3 m-3





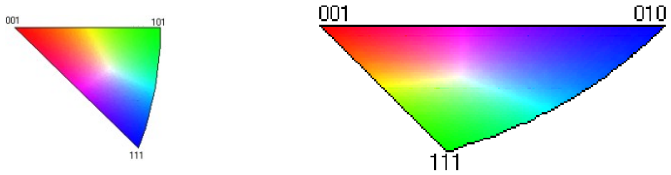
La_2O_3 m3m



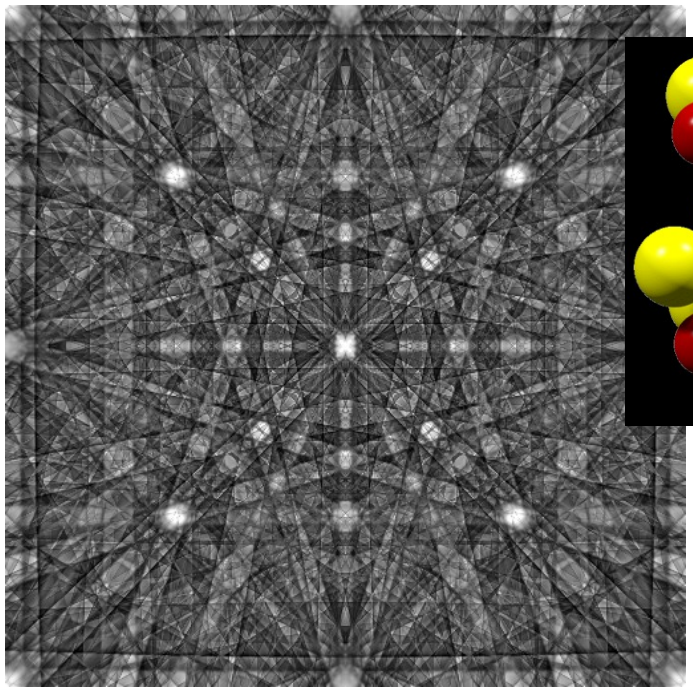
Usually such effects are prevented using a colour key of a higher Laue class.

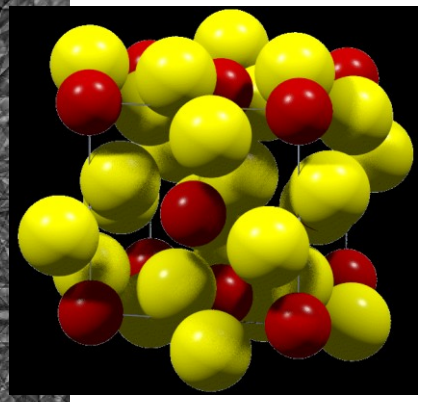
Nevertheless: Crystallographically the light-blue and orange points are not equivalent, i.e. it is only a visual "solution"!

Pseudo-symmetry: cubic FeS_2



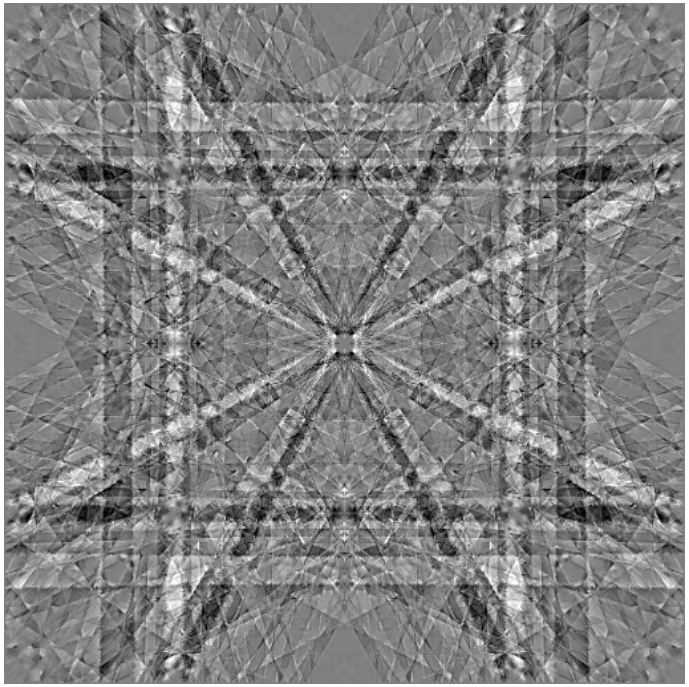
- The pattern simulation shows a 90° rotational symmetry, right?
- The difference plot (between 0° and 90° rotated pattern) reflects only small intensity variations.





{100}, {110} and {111} disappear in difference plot.

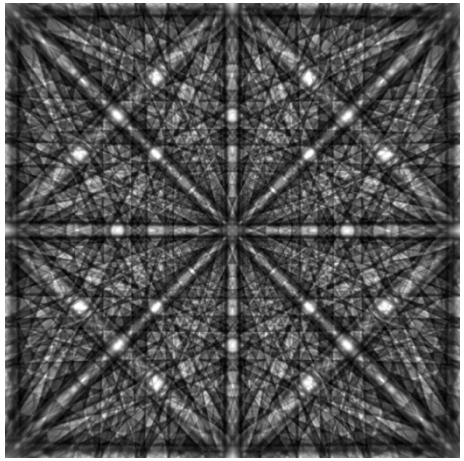
Difference plot between 0° und 90°

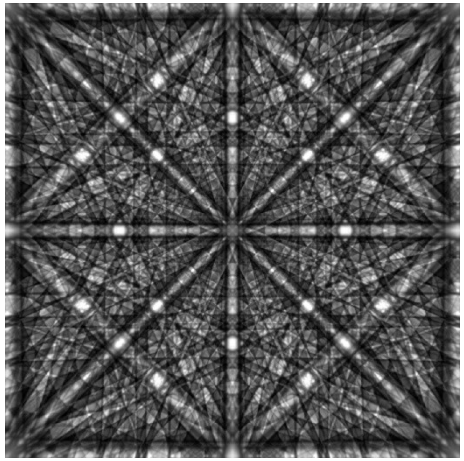


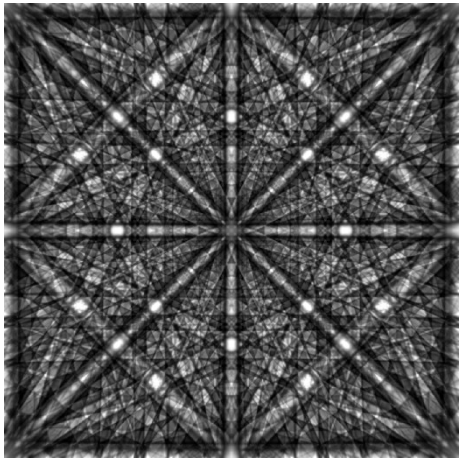
$BaTiO_3$: that is pseudo-symmetry!

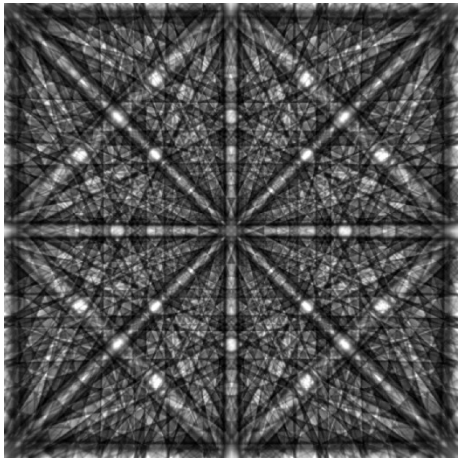
Bundesministerium für Wirtschaft und Technologie

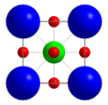
BAM



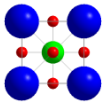




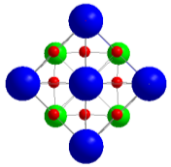




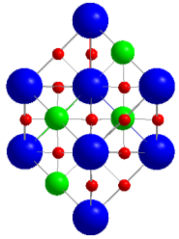
$Pm\bar{3}m$
$a_o = 3.996$ Å



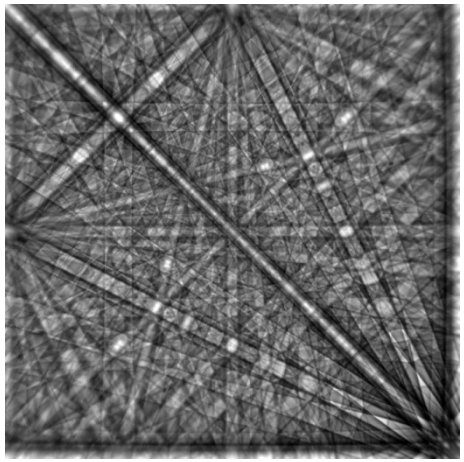
$P4/mmm$
$a_o = 3.982$ Å
$c_o = 4.017$ Å

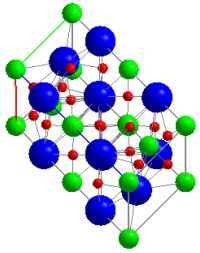


$Amm2$
$a_o = 3.983$ Å
$b_o = 5.675$ Å
$c_o = 5.692$ Å



$R3m$
$a_o = 5.654$ Å
$c_o = 6.954$ Å





$P6_3/mmc$
$a_o = 5.735$ Å
$c_o = 14.050$ Å

Conclusion:

Only the hexagonal phase can be distinguished , but also there a tiny potential of misinterpretation is given by the occurrence of similar bands.

EBSD and crystallography

Conclusions

- Even if structures are described in different symmetries, lattice types, crystal systems…
  it does not automatically mean, that they are differentiable by EBSD.
- The "same" crystal structure can appear slightly "distorted" as different modification in different symmetries.
  They are typically impossible to distinguish!
  Examples: $BaTiO_3$, ZrO_2, superstructures like chalcopyrites…
- Rule:
  What you cannot *clearly* differentiate by XRD is impossible by EBSD!

SYMMETRY INHERITANCE

Again…phase transformations

The **phase transformation in steel** is of high practical relevance and therefore continuously under investigation.

Crystallographically it is **described by different models** where the most important are:

Bain

$\{0\,0\,1\}_\gamma \parallel \{0\,0\,1\}_\alpha \quad \& \quad \langle 0\,1\,0\rangle_\gamma \parallel \langle \bar{1}\,1\,0\rangle_\alpha$

Pitsch

$\{0\,0\,1\}_\gamma \parallel \{1\,1\,0\}_\alpha \quad \& \quad \langle \bar{1}\,1\,0\rangle_\gamma \parallel \langle \bar{1}\,1\,1\rangle_\alpha$

Nishiyama–Wassermann

$\{1\,1\,1\}_\gamma \parallel \{1\,1\,0\}_\alpha \quad \& \quad \langle \bar{1}\,1\,0\rangle_\gamma \parallel \langle 0\,0\,1\rangle_\alpha$

Kurdjumov–Sachs

$\{1\,1\,1\}_\gamma \parallel \{1\,1\,0\}_\alpha \quad \& \quad \langle \bar{1}\,1\,0\rangle_\gamma \parallel \langle \bar{1}\,1\,1\rangle_\alpha$

Comparing the different crystallographic descriptions of parallel lattice planes and directions one gets the impression that the steels investigated were of totally different nature.

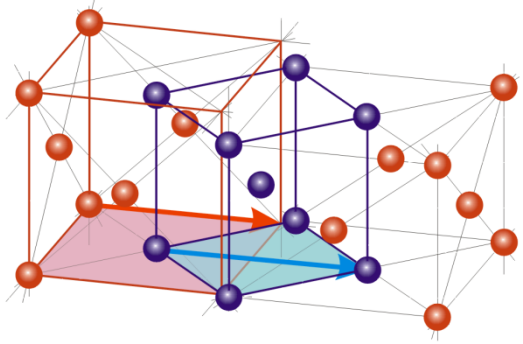
Transformation symmetries

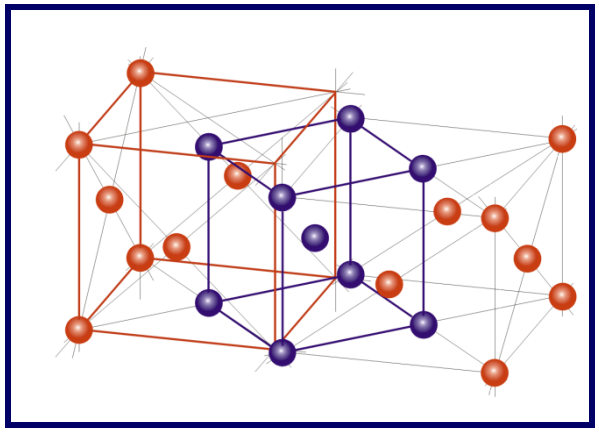
Bundesministerium für Wirtschaft und Technologie

BAM

Bain

$\{001\}_\gamma \,||\, \{001\}_\alpha \quad \langle 010\rangle_\gamma \,||\, \langle -110\rangle_\alpha$

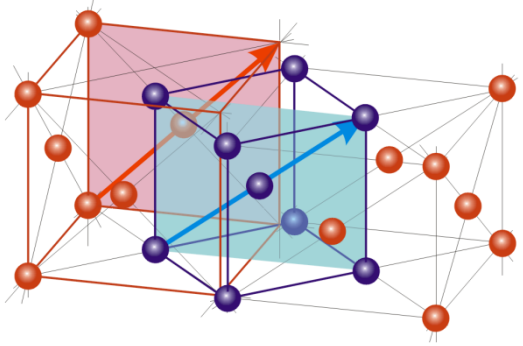




but…where is the problem?
All fits perfect…

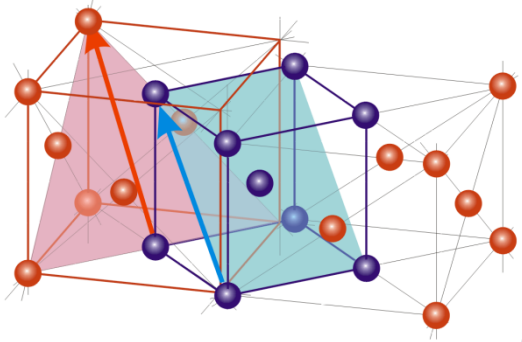
Pitsch

$\{100\}_\gamma \,||\, \{110\}_\alpha \quad \langle 011\rangle_\gamma \,||\, \langle -111\rangle_\alpha$



Nishiyama-Wassermann

$\{111\}_\gamma \,||\, \{011\}_\alpha \quad \langle -1\text{-}12\rangle_\gamma \,||\, \langle -001\rangle_\alpha$

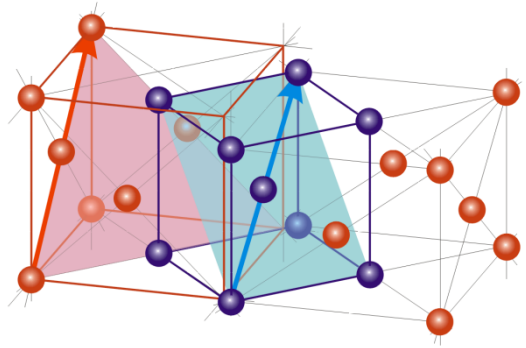


The transformation lattice is not cubic!

- Lattice deformation are required
- …but then neither the atoms nor the lattice planes fit well

Kurdjumov-Sachs

$\{111\}_\gamma \,||\, \{011\}_\alpha \quad \langle -101\rangle_\gamma \,||\, \langle -1\text{-}11\rangle_\alpha$



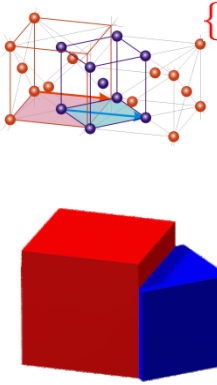
Atomic scale

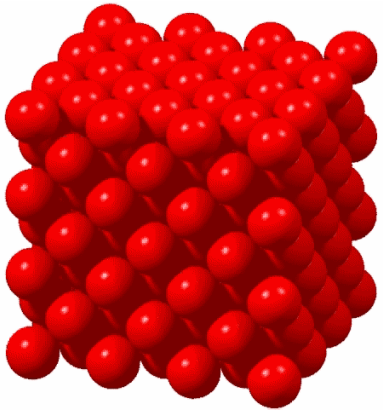
Bundesministerium für Wirtschaft und Technologie

BAM

Bain

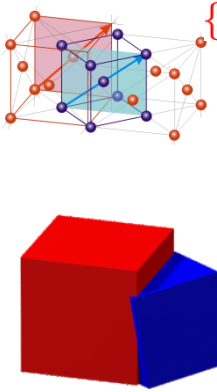
$\{0\,0\,1\}_\gamma \| \{0\,0\,1\}_\alpha \quad \langle 0\,1\,0\rangle_\gamma \| \langle \bar{1}\,1\,0\rangle_\alpha$

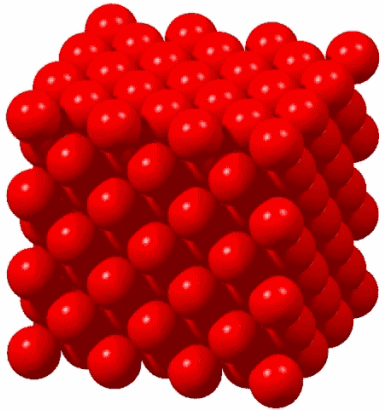




Pitsch

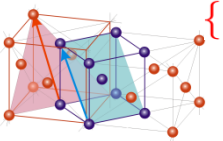
$\{0\,0\,1\}_\gamma \| \{0\,1\,1\}_\alpha \quad \langle \bar{1}\,1\,0\rangle_\gamma \| \langle 1\,\bar{1}\,1\rangle_\alpha$

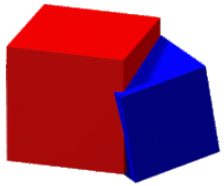


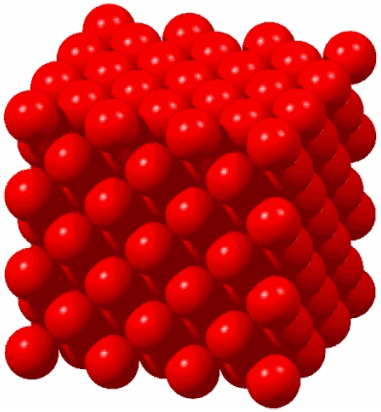


Nishiyama-Wassermann

$\{1\,1\,1\}_\gamma \| \{0\,1\,1\}_\alpha \quad \langle \bar{1}\,1\,0\rangle_\gamma \| \langle 1\,0\,0\rangle_\alpha$

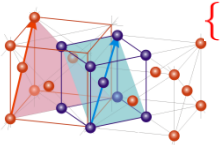


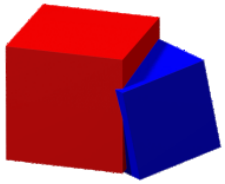


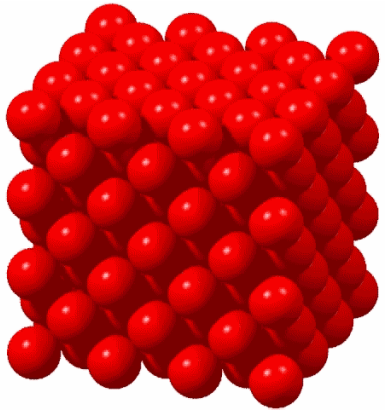


Kurdjumov-Sachs

$\{1\,1\,1\}_\gamma \| \{0\,1\,1\}_\alpha \quad \langle \bar{1}\,1\,0\rangle_\gamma \| \langle 1\,\bar{1}\,1\rangle_\alpha$





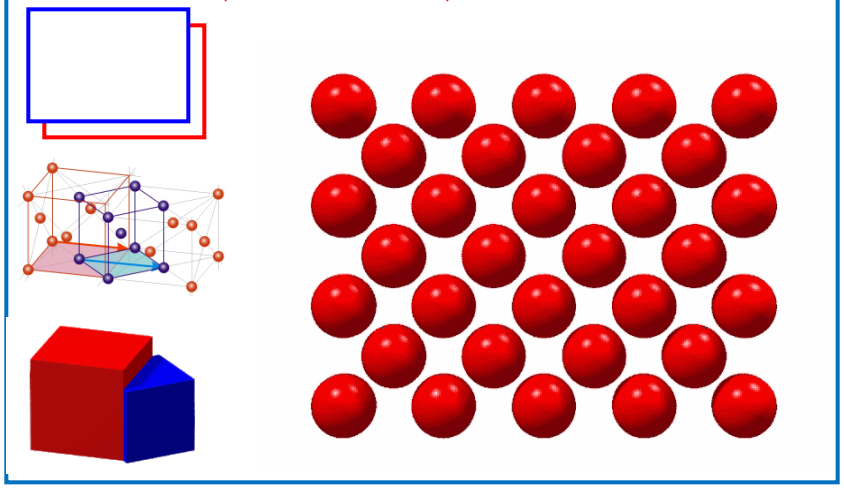


Phase boundary characteristics

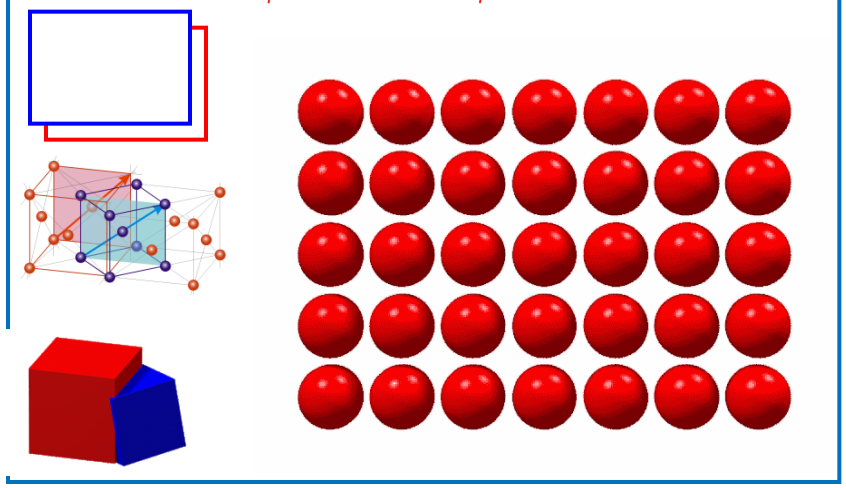
Bundesministerium für Wirtschaft und Technologie

BAM

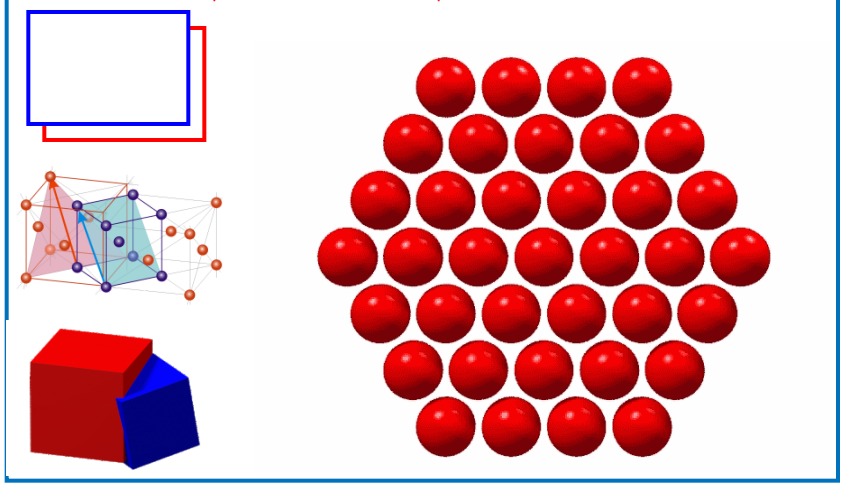
Bain: $\{001\}_\gamma \parallel \{001\}_\alpha \quad \langle 010\rangle_\gamma \parallel \langle \text{-}110\rangle_\alpha$



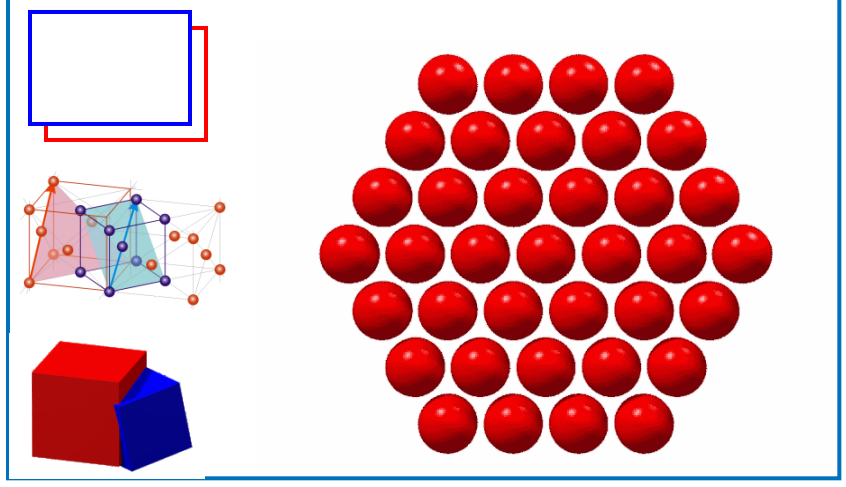
Pitsch: $\{100\}_\gamma \parallel \{110\}_\alpha \quad \langle 011\rangle_\gamma \parallel \langle \text{-}111\rangle_\alpha$



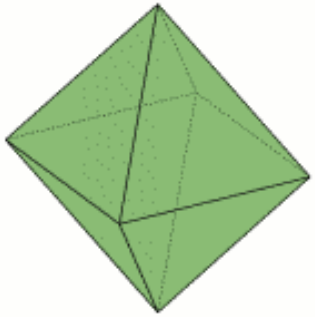
N-W: $\{111\}_\gamma \parallel \{011\}_\alpha \quad \langle \text{-}110\rangle_\gamma \parallel \langle \text{-}100\rangle_\alpha$

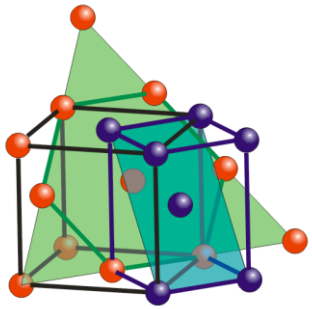


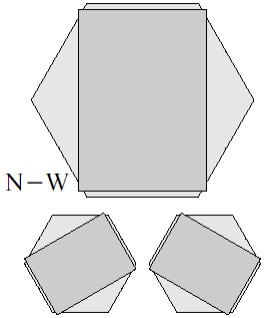
K-S: $\{111\}_\gamma \parallel \{011\}_\alpha \quad \langle \text{-}101\rangle_\gamma \parallel \langle \text{-}1\text{-}11\rangle_\alpha$



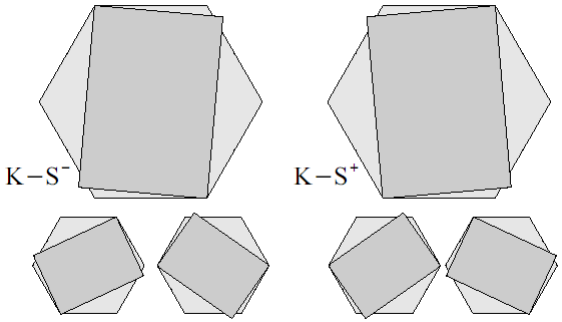
Transformation pole figures



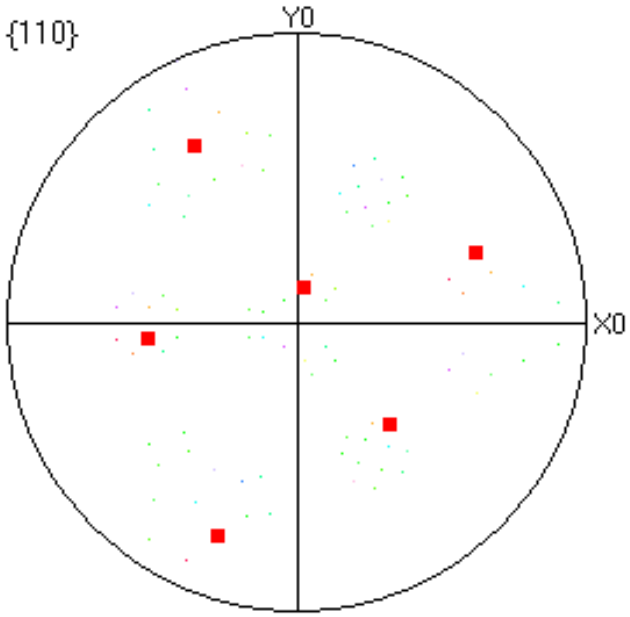




3×4=12



3×2×4=24



Phase transformations generates a distinct number of different but equivalent crystal orientations. These are called *variants*.

The number of this variants depends on the crystal symmetry of both phases.

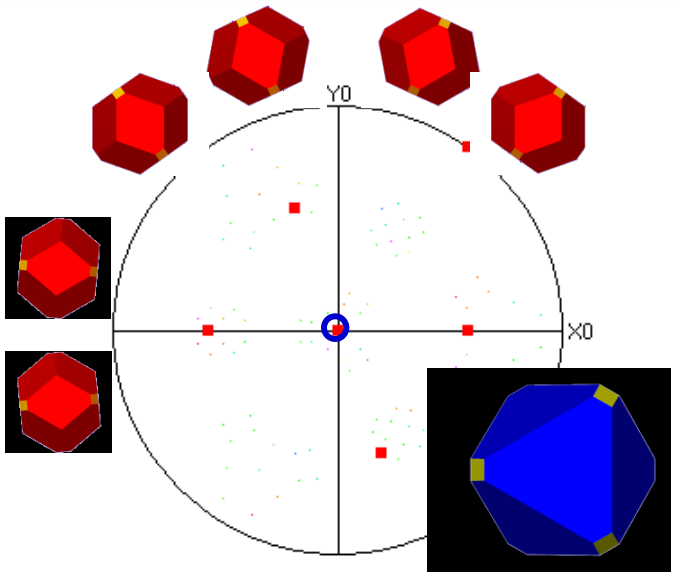
In order to simulate a pole figure {hkl} each variant must be considered by its complete pole distribution:

$$\text{Number}_{\{hkl\}} = \text{Number}_{\text{variants}} \times \text{Multiplicity}_{\{hkl\}}$$

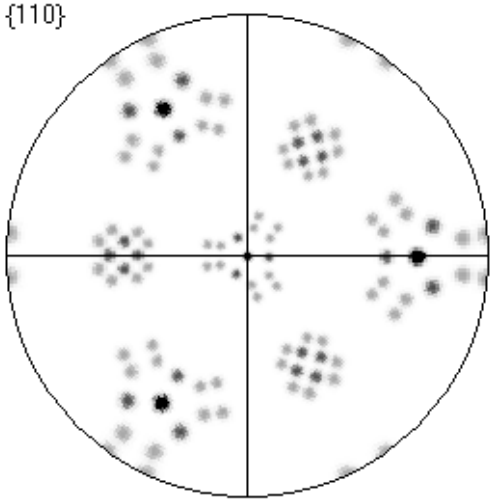
Bundesministerium für Wirtschaft und Technologie

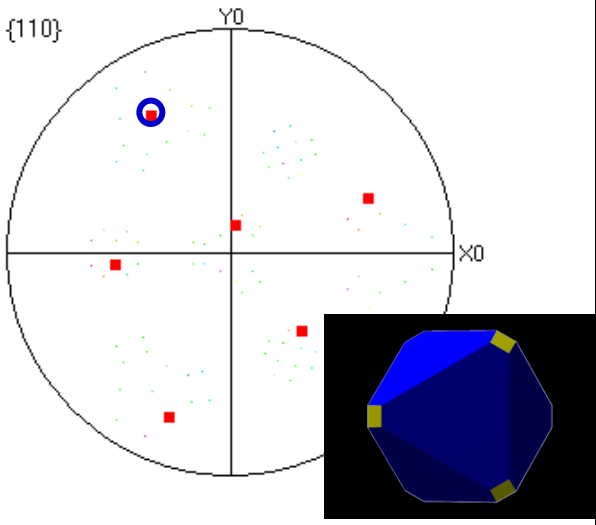
BAM

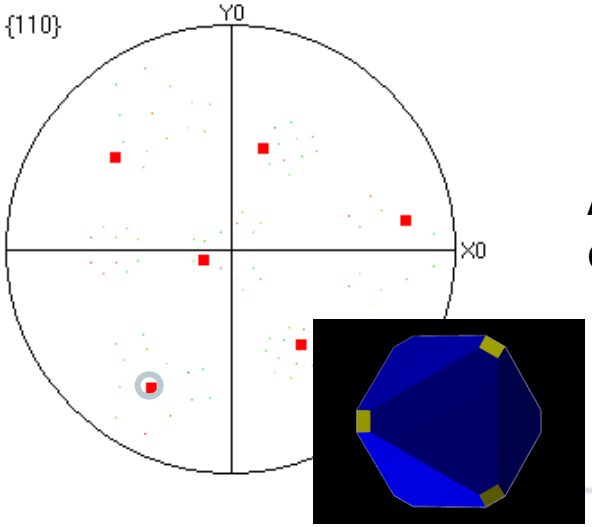
Pole figures related to $\{111\}_{fcc}$



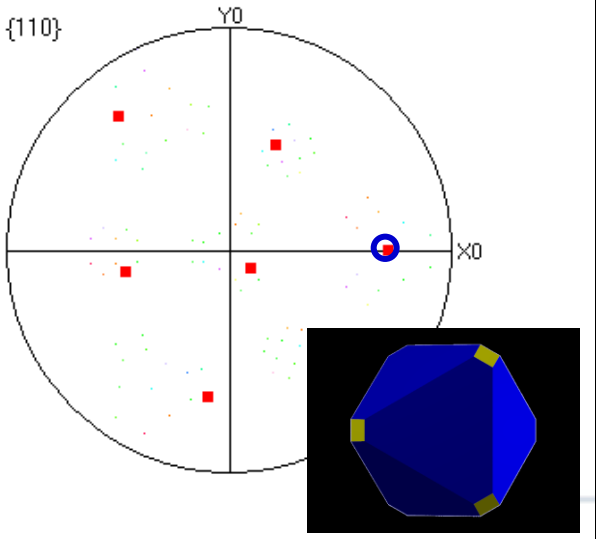
overlay







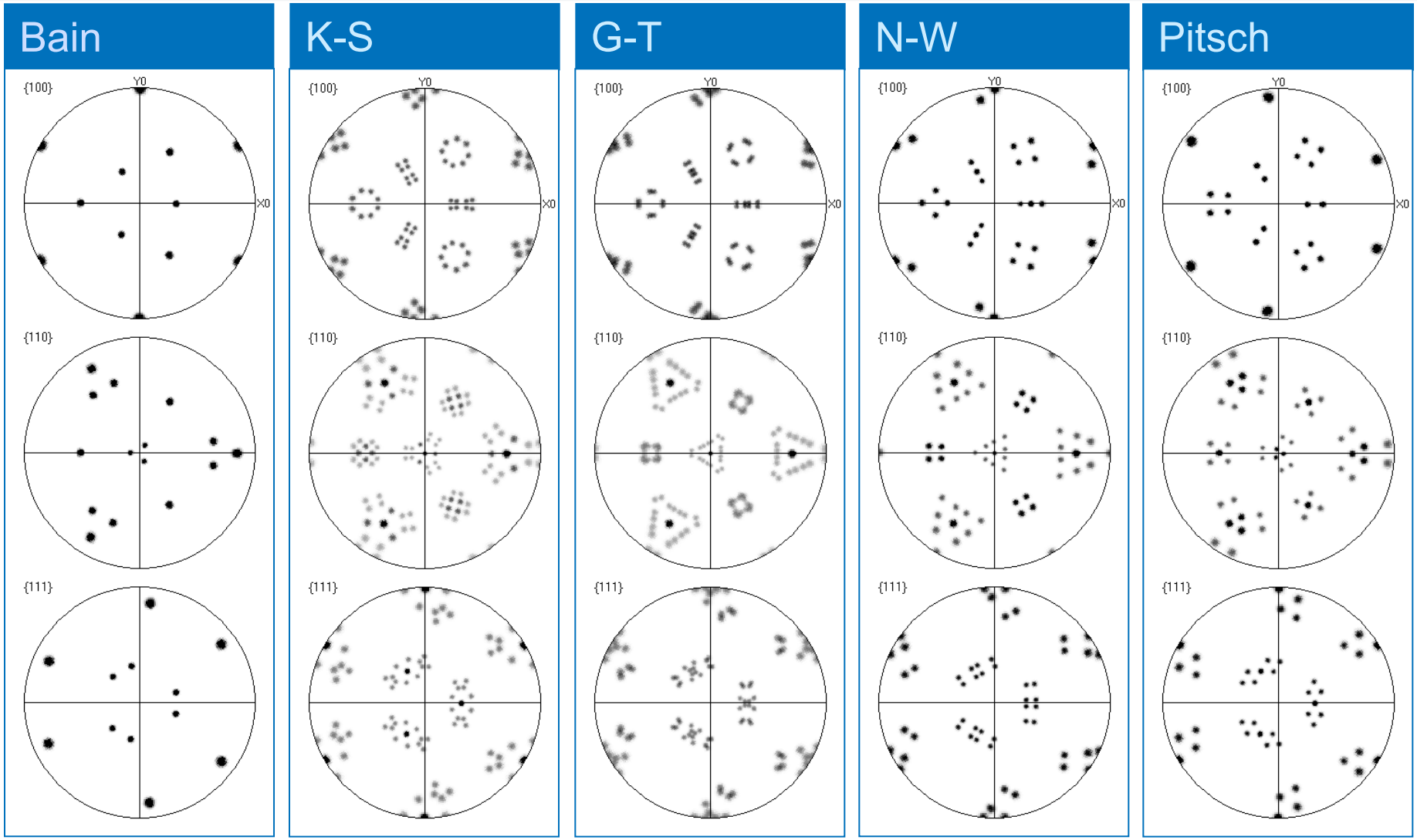
Automatic simulations consider the **multiple occupations** in pole figures.



Transformation pole figures

Bundesministerium für Wirtschaft und Technologie

BAM



Transformation pole figures

Consequences:

One needs to know the symmetry of both phases in order to generate transformation pole figures.

The **lattice description** can highly **irritate** regarding the real transformation process since this still happen on the atomic level of course.

Remember: lattice planes and vectors are commonly not related to atomic positions.
They only describe the translation symmetry of the motif which can contain thousands of atoms, e.g. in proteins.

Example: hcp (hexagonal closed-packed)
Even for this very simple structure not any atom is sitting at the origin of the unit cell!

SAMPLE SYMMETRY

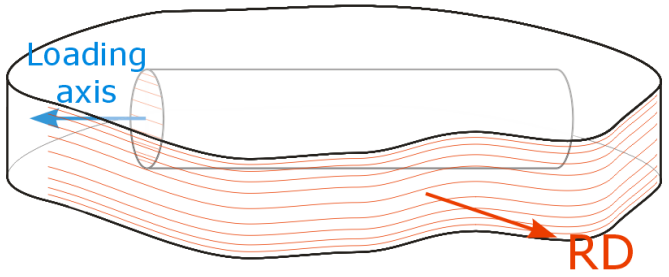
Sample symmetry

This term is often misleading since the sample shape alone is not automatically linked to the microstructure, texture, mechanical or physical properties etc.

See also: process symmetry

Example:

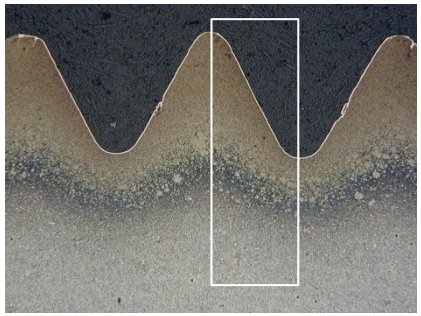
cylindrical sample from a rolled sheet



Sample symmetry:

Can be applied if samples are rotationally symmetric (2…∞), orthotropic (mmm), or mirror-symmetric (m) in order

- to reduce the experimental or analytical effort *(e.g. measuring less orientation data)*, or
- to increase the statistical relevance of data *(coarse grain material, i.e. many grains and not many single EBSD measurements)*



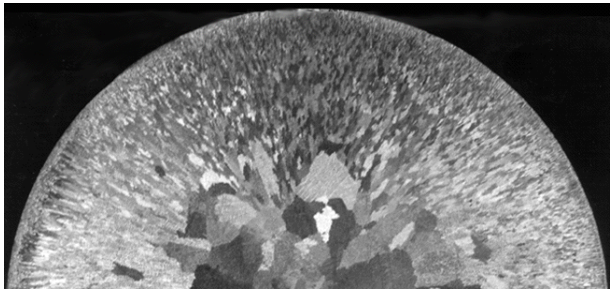
Correct alignment or re-adjustment necessary!

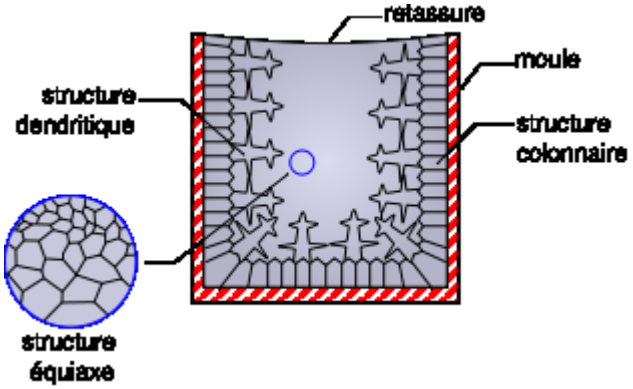
Reference coordinate system

A fixed reference coordinate system makes no sense since it is moving…?

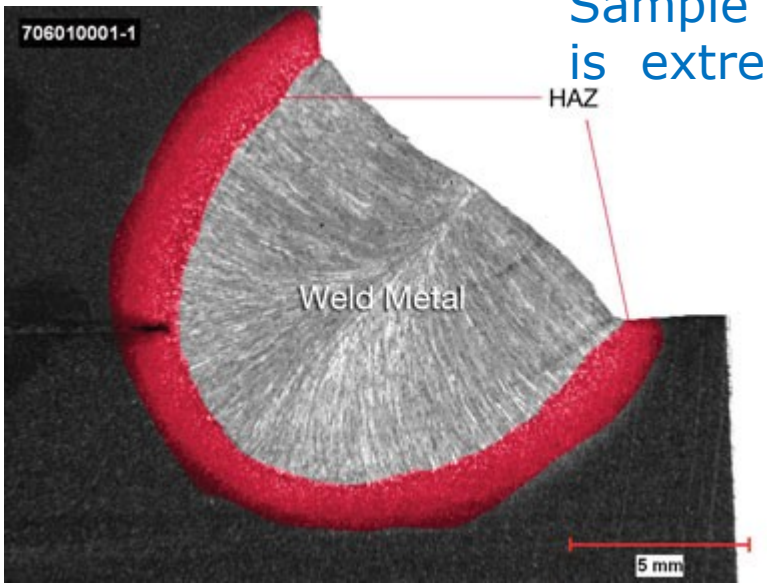
Examples:

Casting,
Wire drawing,
Welding,
Corrosion
…





Sample (area) selection is extremely important!



Conclusions are very difficult or only representative for the specific area investigated.

Process symmetries

Bundesministerium für Wirtschaft und Technologie

BAM

Whereas the sample symmetry actually only describes the sample shape, the **process symmetry** gives some information about the assumed symmetry of external influences **during sample treatment**.

Process symmetry

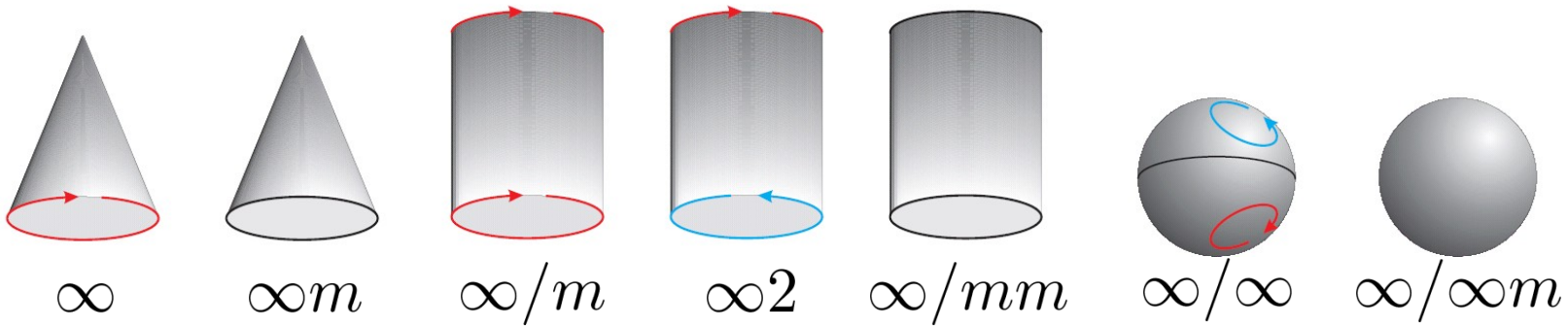
- De-facto every manufacturing process has a specific symmetry.
- The process symmetry should have the same or higher symmetry than the sample.
- Especially for high-symmetric materials (e.g. cubic) the process symmetry commonly reduces the “effective” crystal symmetry.
- The final symmetry is given by the intersection of all symmetries: crystal symmetry, process symmetry and sample symmetry.
- Requires a sufficient alignment of the symmetry axes.

Continuous symmetry groups

Bundesministerium für Wirtschaft und Technologie

BAM

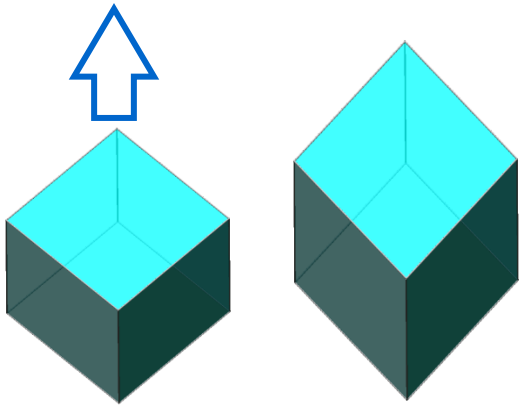
Very often it is recommended to consider symmetries coming from the used process. To this end the so-called ***continuous*** or *Neumann* ***groups*** (Curie's principle) have been introduced.



The symmetry elements of any physical property of a crystal must include all symmetry elements of the point group.

Example: Tensile test of a [111]-oriented single crystal

caused by the tensile load (∞/mm) all fourfold and threefold axes disappear (except of the tensile axis) and the crystal is no more cubic but trigonal.



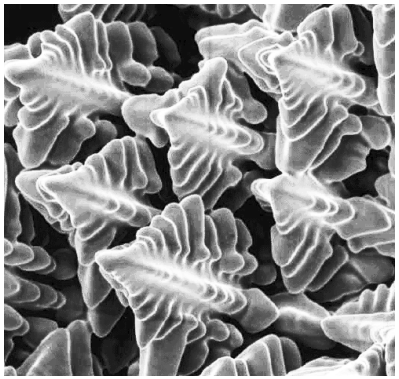
Sample geometry:

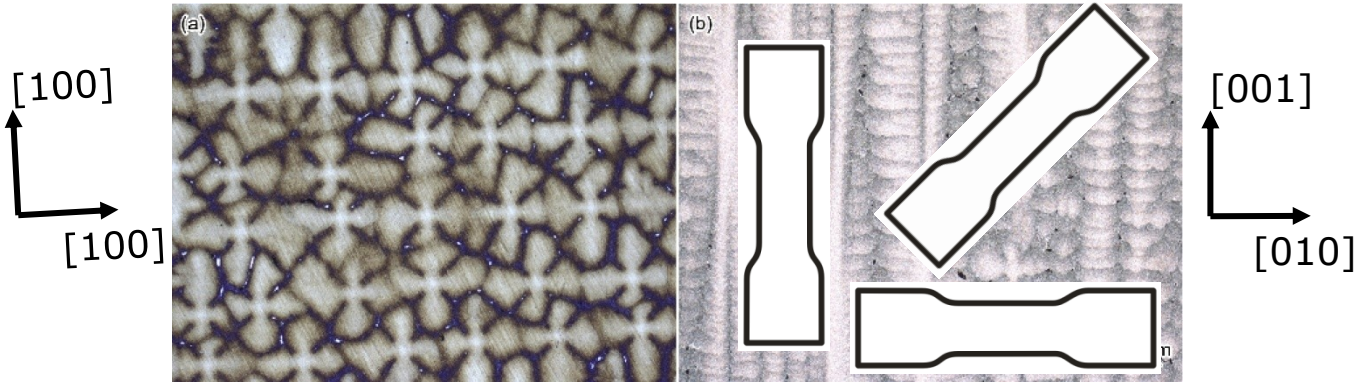
Cubic means not always…cubic

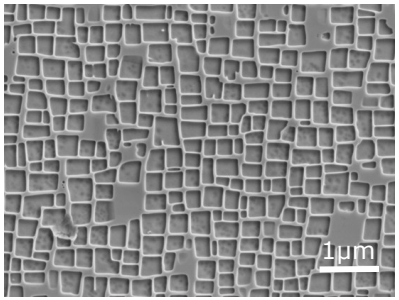
Bundesministerium für Wirtschaft und Technologie

BAM

- "**single-crystalline**" Ni-based superalloy is a casted material, and consists of millions of **dendrites with a** dimension of e.g. 0.1x0.1x300mm, i.e. the dendrites have a **form factor of 1000** and higher
- Strong chemical **gradients** from the dendrite center to the interdendritic region
- The "single crystal" consists of **two** cubic **phases**: γ (fcc) and an ordered γ'







Conclusion:

One should not use [001]-solidified crystals in order to compare the anisotropy in mechanical properties of the macroscopic [001], [011] and [111] since already [100] is no more equivalent to [001]…although crystallographically there are still cubic phases and everything is practically well aligned.

Sample alignment accuracy in SEM

Bundesministerium für Wirtschaft und Technologie

BAM

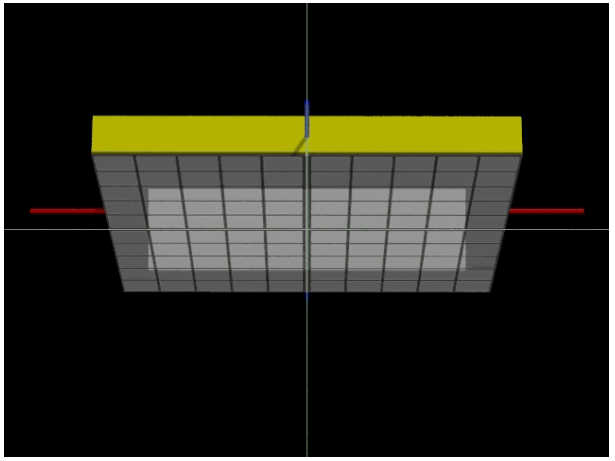
- Often one observes surface contamination in SEM during electron bombardment

negativ: charging and image drift, a new measurement is not comparable (scattering in the contamination layer)

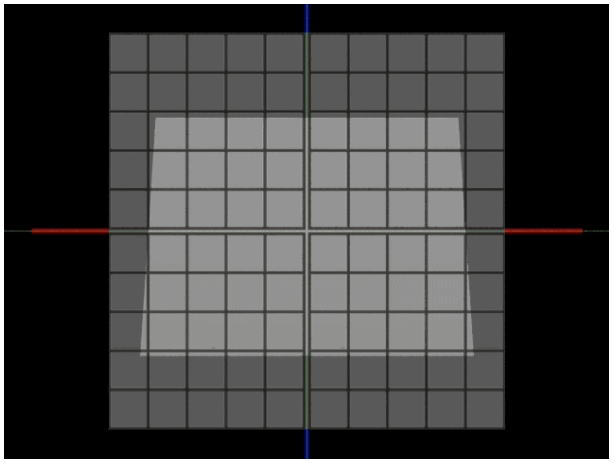
positiv: Distortion effects become visible caused by electron optic design, but mainly they are the result of misalignment of the sample

3° out of plane

View from the cathode



View from the camera



SE image at tilted sample

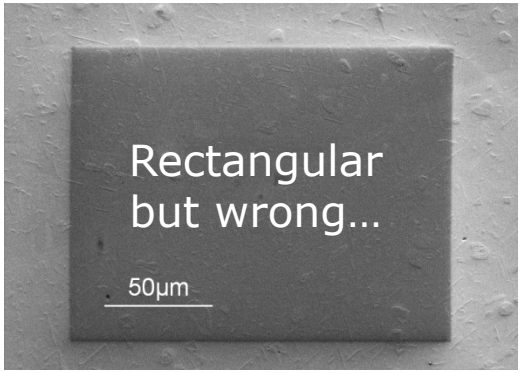
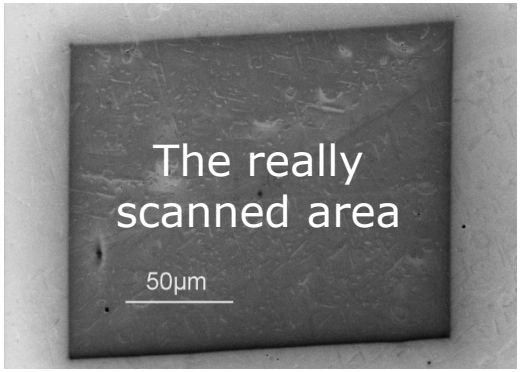


Image at horizontal sample



Sample alignment accuracy in SEM

Bundesministerium für Wirtschaft und Technologie

BAM

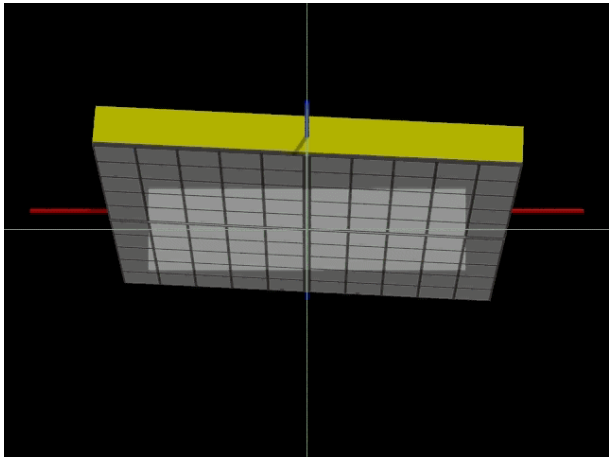
- Often one observes surface contamination in SEM during electron bombardment

negativ: charging and image drift, a new measurement is not comparable (scattering in the contamination layer)

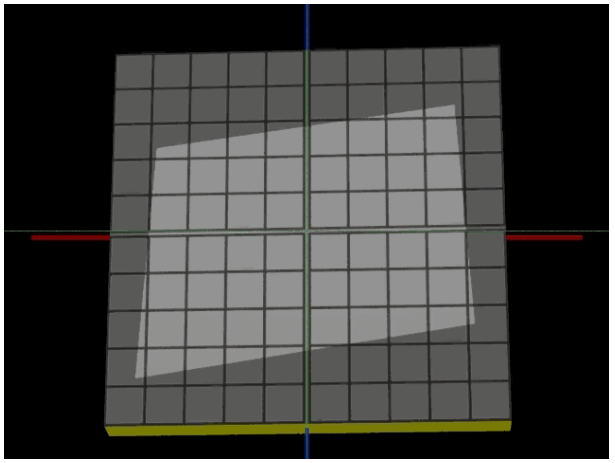
positiv: Distortion effects become visible caused by electron optic design, but mainly they are the result of misalignment of the sample

3° out of plane

View from the cathode



View from the camera



SE image at tilted sample

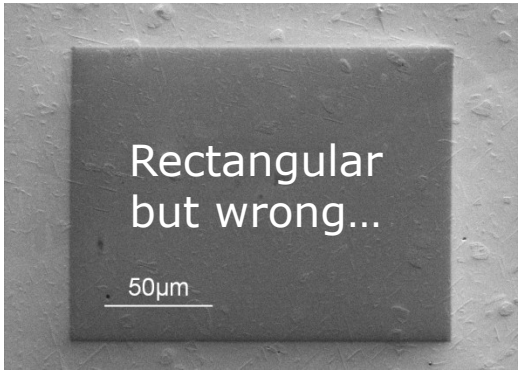
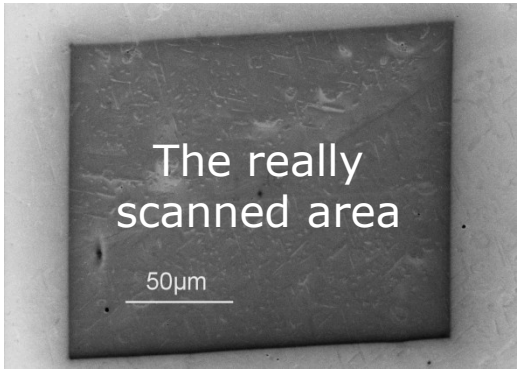


Image at horizontal sample



Summary

- The consideration of **symmetry** for crystalline samples does not only include **crystal** symmetry of different phases but also **sample** and **process** symmetry
- The **lowest symmetry** (crystal, sample, process) finally **decides** about the usable simplification (Neumann's principle).
- **Pseudo-symmetries** are can be caused by a similar **lattice metric**, but also by the **crystal structure** (similar scattering atoms), or simply by a similar **diffraction signal**.
- **Small deviations** from the real symmetry – i.e. pseudo-symmetries – disturb the data acquisition, but from the practical point of view their impact on physical properties **are often of low importance**.
  Commonly, a change to the pseudo-symmetry is the best and most efficient solution.
- If significant advantages exist, e.g. the determination of the polarity of lattice planes, or the prevention of systematic misindexings (pyrite, quartz, or in multiphase materials) **advanced tools are required** which are nowadays not available.