Karlsruhe Institute of Technology

IAM
Institute for Applied Materials

Plasticity

Lecture for “Mechanical Engineering” and “Materials Science and Engineering”
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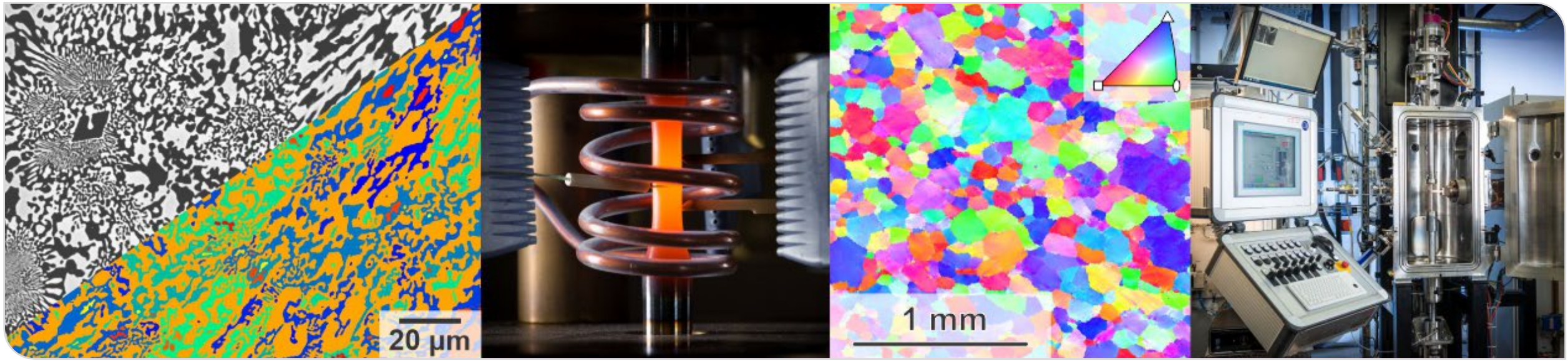
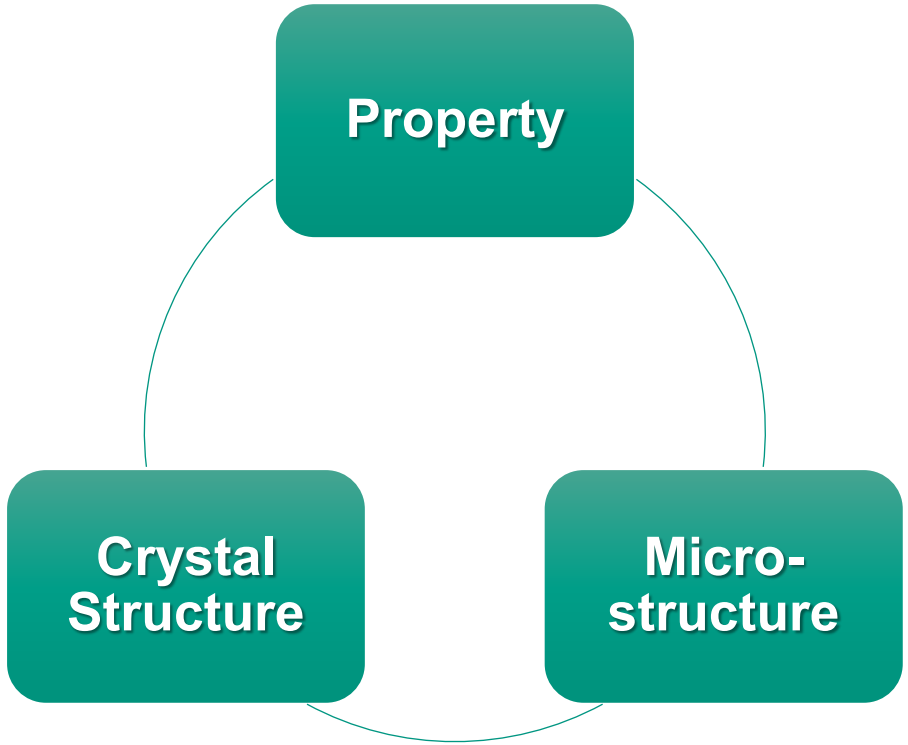


Topics

- Structure-Microstructure-Property Relationships
- Definitions and Terms
  - Crystal
  - Crystal Structure
  - Lattice and Atomic Basis
  - Primitive and Conventional Cell
  - Crystal System
  - Bravais Types of Lattices
  - Indexing of Directions and Planes
  - Symmetry
  - Point Groups, Space Groups, Wykoff Positions, International Tables
- Common Short Notations
  - Prototypes
  - Strukturbericht Designation
- Important Crystal Structures

Structure-Microstructure-Property Relationship



All features determined by the thermodynamic equilibrium state

All features that are not determined by thermodynamic equilibrium state

Of course, **most features discussed in this class are related to deviations (defects) from thermodynamic ground state**! Nevertheless, the description of deviations needs a **proper understanding of the ideal state**. Hence, crystallography provides the basis for any defect classification.

Nobel Prize for W.C. Röntgen in 1901

- **Wilhelm Conrad Röntgen discovers X-rays** which are necessary to investigate crystal structures in metallic materials due to their wavelength and interaction with the atoms (or more precise with the electrons of the atoms).

W. C. Röntgen:
„Ueber eine neue Art von Strahlen. Vorläufige Mitteilung.“ Sitzungsberichte d. Würzburger physik.-med. Ges. Würzburg (1895) 132-141
https://de.wikipedia.org/wiki/Wilhelm_Conrad_R%C3%B6ntgen#/media/File:Roentgen2.jpg
https://de.wikipedia.org/wiki/Wilhelm_Conrad_R%C3%B6ntgen#/media/File:X-ray_by_Wilhelm_R%C3%B6ntgen_of_Albert_von_K%C3%B6lliker%27s_hand_-_18960123-02.jpg

Nobel Prize for M. v. Laue in 1914

- **Max von Laue**, **Walter Friedrich**, and **Paul Knipping** discover and successfully describe the diffraction of X-ray beams in crystals.

- The physical implication of this experiment is that X-rays are waves. Furthermore, they provide a versatile tool for analysis of crystal structures.

Max von Laue

Diffraction pattern of a ZnS (sphalerite) along a [100] zone axis

W. Friedrich, P. Knipping & M. v. Laue:
„Interferenz-Erscheinungen bei Röntgenstrahlen“ Sitzungsberichte d. Königl. Bay. Akad. d. Wiss. 14 (1912) 303-322
https://de.wikipedia.org/wiki/Max_von_Laue#/media/File:Bundesarchiv_Bild_183-U0205-502,_Max_von_Laue.jpg

Definition: Crystal

- Modern version (that includes aperiodic structures, like quasi crystals):

  A material is a crystal if it has **essentially a sharp diffraction** pattern. The word essentially means that most of the intensity of the diffraction is concentrated in relatively sharp Bragg peaks, besides the always present diffuse scattering.

- Former version:

  A crystal consists of a **3D periodic arrangement of atoms**. Hence, its structure can be **described by a small volume translated along the basis vectors**.

http://reference.iucr.org/dictionary/Crystal

Nobel Prize for D. Shechtman in 2011

- The modification of the definition of crystals traces back to the discovery of quasicrystals by Dan Shechtman. These are crystals with aperiodic structures exhibiting distinct diffraction patterns with symmetries incommensurate with translation symmetry.

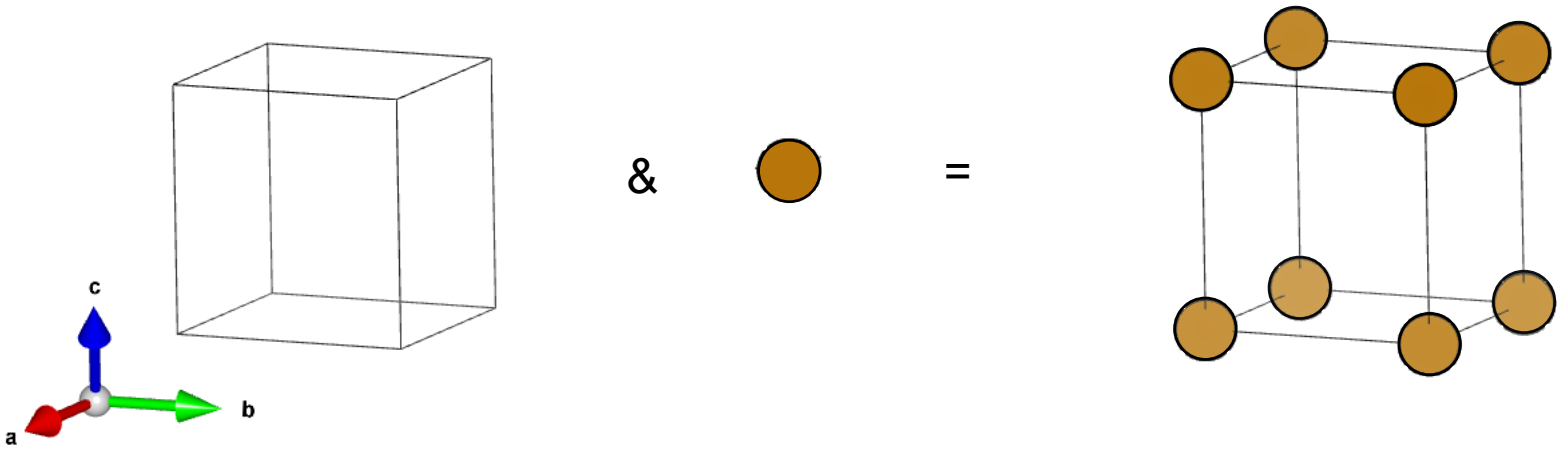
Symmetry elements and selected area electron diffraction pattern of an icosahedral phase

Dan Shechtman

D. Shechtman, et al.:
„Metallic Phase with Long-Range Orientational Order and No Translational Symmetry“ Phys. Rev. Lett. 53 (1984) 1951-1953
https://de.wikipedia.org/wiki/Dan_Shechtman#/media/File:Nobel_Prize_2011-Nobel_interviews_KVA-DSC_8039.jpg

Definition: Crystal Structure

- The fundamental principle of crystallography is to split the information about the crystal into:
  crystal = lattice & basis



http://reference.iucr.org/dictionary/Crystal

Definition: Crystal Structure

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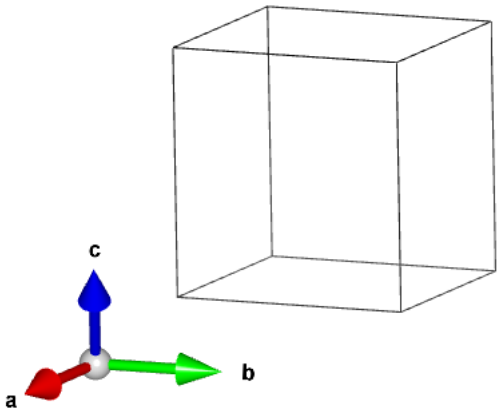
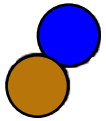


&



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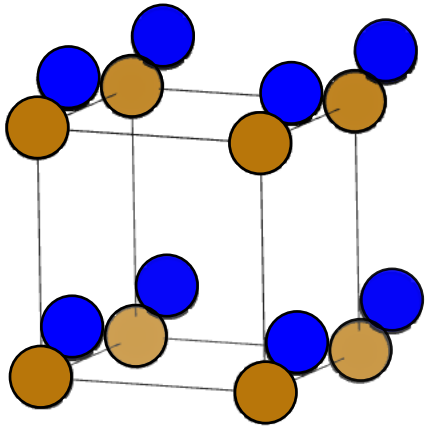


The same point lattice can obviously lead to different crystal structures. „**face centered cubic**“ is therefore an imprecise description for the crystal structure of many metals since it **only contains information about the point lattice**. The diamond structure of many semi-conductors is also face centered cubic!

http://reference.iucr.org/dictionary/Crystal

Definition: Crystal Structure

- **Point Lattice**:

  The lattice is a 3D periodic arrangement of points. Points are objects without geometrical attribute, like length, area, volume, etc.

- **Atomic Basis**:

  Motive of atoms or groups of atoms which are placed on each and every point of the lattice to form the crystal structure.

Definition: Unit Cell

- **Unit cell**: The unit cell is the **parallelepiped** built from the three basic vectors $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ in real space.
- Its **volume** is given by the scalar triple product:

$$V = (\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{c}$$

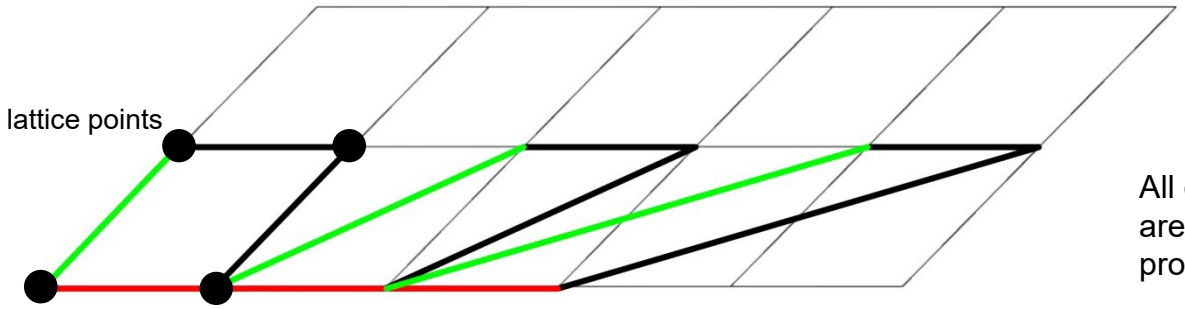
- The **ideal crystal** is obtained by **perfect, infinite translation** of the unit cell along all basis vectors.

https://dictionary.iucr.org/Unit_cell

Definition: Primitive Cells

- **Primitive cell**: Primitive cells only contain a single lattice point.

  Hence, the primitive cell has the **smallest volume** to describe the entire crystal. Furthermore, there is an **infinite number of equivalent primitive cells**:



All depicted unit cells are primitive and are of the same volume (given by the product of base length and height).

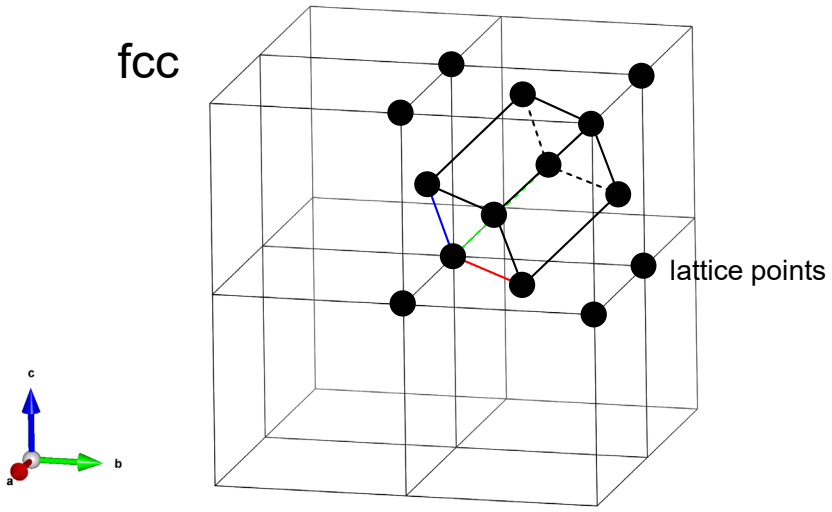
http://reference.iucr.org/dictionary/Primitive_cell

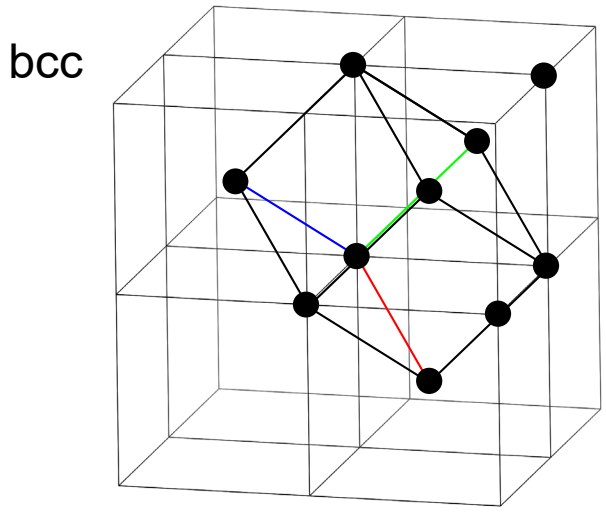
Definition: Conventional Cell

- Crystallography in modern sense intensively focuses on symmetry considerations.
- Hence, the conventional cell is the unit cell obeying the following conditions:
  - Its basis vectors define a **right-handed axial setting**.
  - Its **edges are along symmetry directions** of the lattice.
  - It is the **smallest cell compatible with the above condition**.

http://reference.iucr.org/dictionary/Conventional_cell

Example: Primitive vs. Conventional Cell





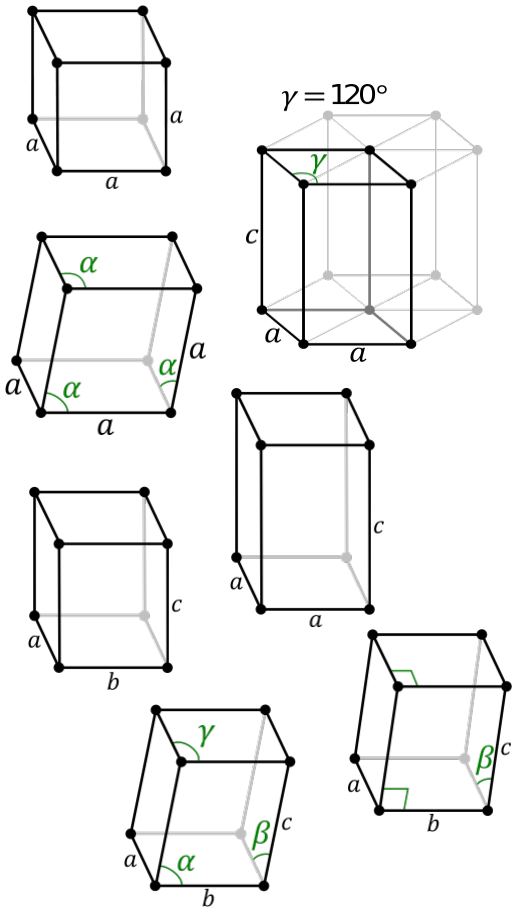
	Conventional	Primitive
Description	fcc	trigonal
	$a[100], a[010], a[001]$	$^a/_2\,[110], {}^a/_2\,[011], {}^a/_2\,[101]$
	$a = b = c,$ $\alpha = \beta = \gamma = 90°$	$a' = b' = c',$ $\alpha' = \beta' = \gamma' = 60°$
No. of lattice points	$8 \cdot 1/8 + 6 \cdot 1/2 = 4$	1
Volume	a^3	$a^3/4$

	Conventional	Primitive
Description	bcc	trigonal
	$a[100], a[010], a[001]$	$^a/_2\,[\bar{1}11], {}^a/_2\,[1\bar{1}1], {}^a/_2\,[11\bar{1}]$
	$a = b = c,$ $\alpha = \beta = \gamma = 90°$	$a' = b' = c',$ $\alpha' = \beta' = \gamma' = 109.5°$
No. of lattice points	$8 \cdot 1/8 + 1 = 2$	1
Volume	a^3	$a^3/2$

Definition: Crystal System

- The crystal systems are the **seven relevant right-handed axial settings in crystallography**. Relevant refers to the definition of the conventional cell.

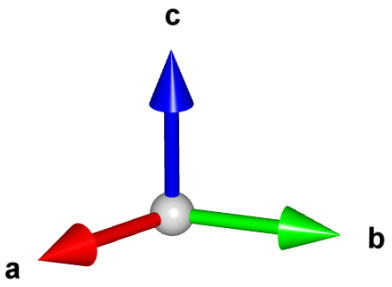
Crystal System	Parameters
triclinic	$a \neq b \neq c, \alpha \neq \gamma \neq \beta$
monoclinic	$a \neq b \neq c, \alpha = \gamma, \beta = 90°$
orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90°$
tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90°$
trigonal	$a = b = c, \alpha = \beta = \gamma \neq 90°$
hexagonal	$a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$
cubic	$a = b = c, \alpha = \beta = \gamma = 90°$



In literature, the rhombohedral system is often mentioned as crystal system. It is not an additional crystal system but belongs to the trigonal system. It is a special type of centered hexagonal system.

https://dictionary.iucr.org/Crystal_system
https://en.wikipedia.org/wiki/Crystal_system#Bravais_lattices

Definition: Crystal System



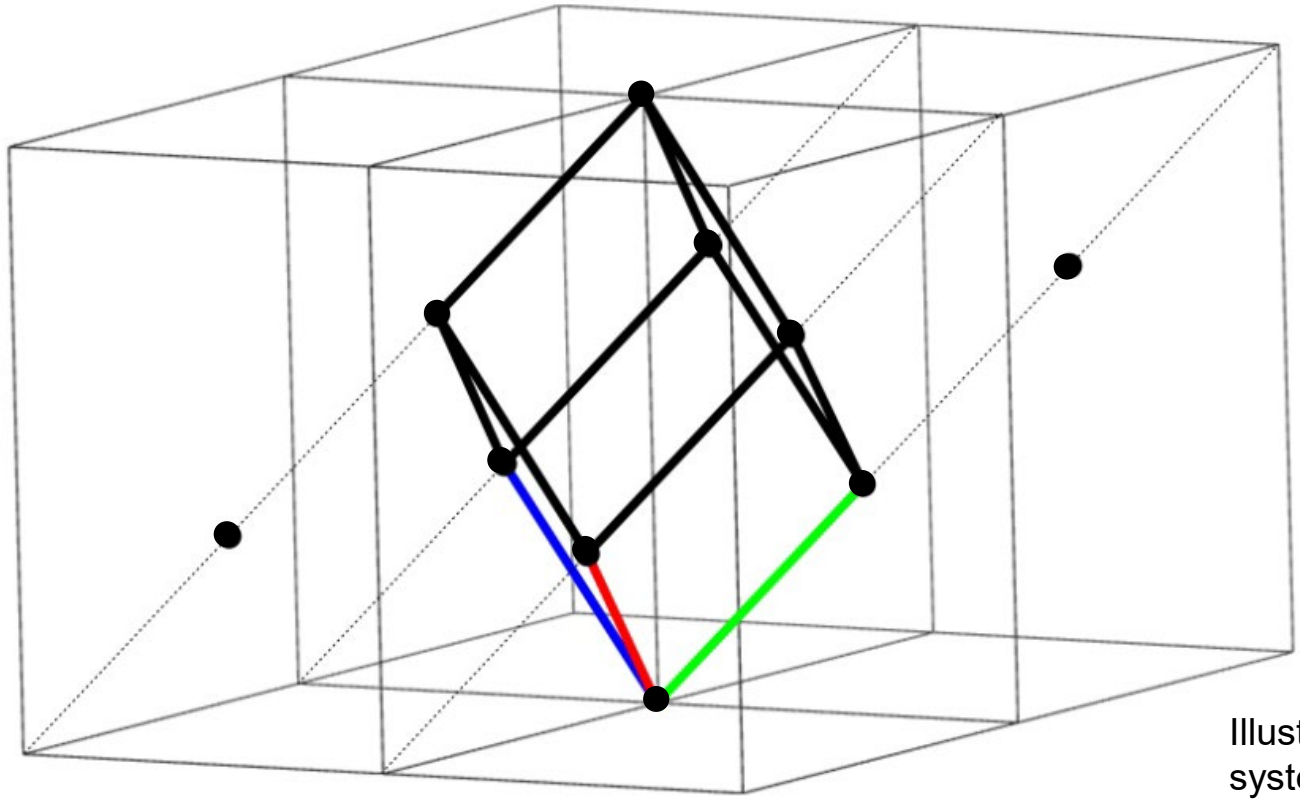
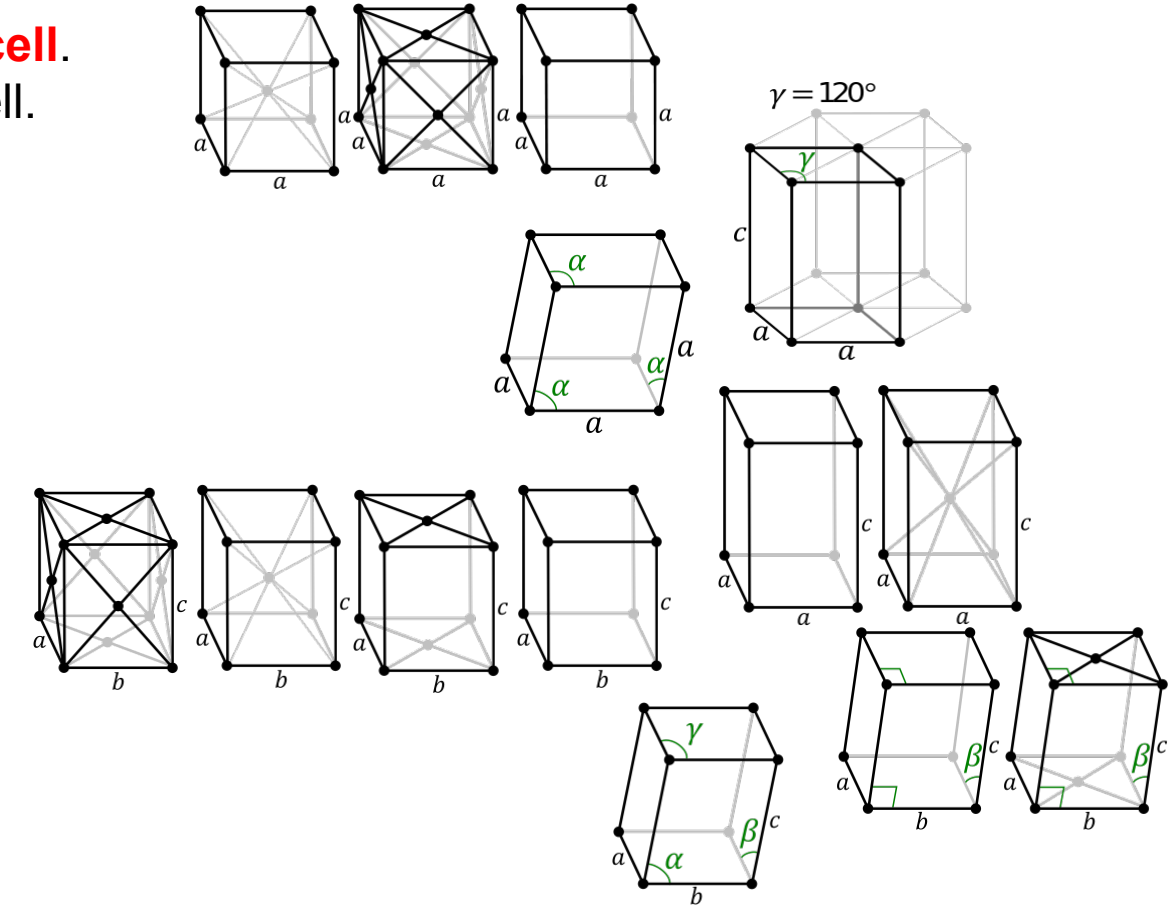


Illustration of the trigonal crystal system in the rhombohedral setting using a hexagonal cell with “rhombohedral centering”.

Definition: Bravais Types of Lattices

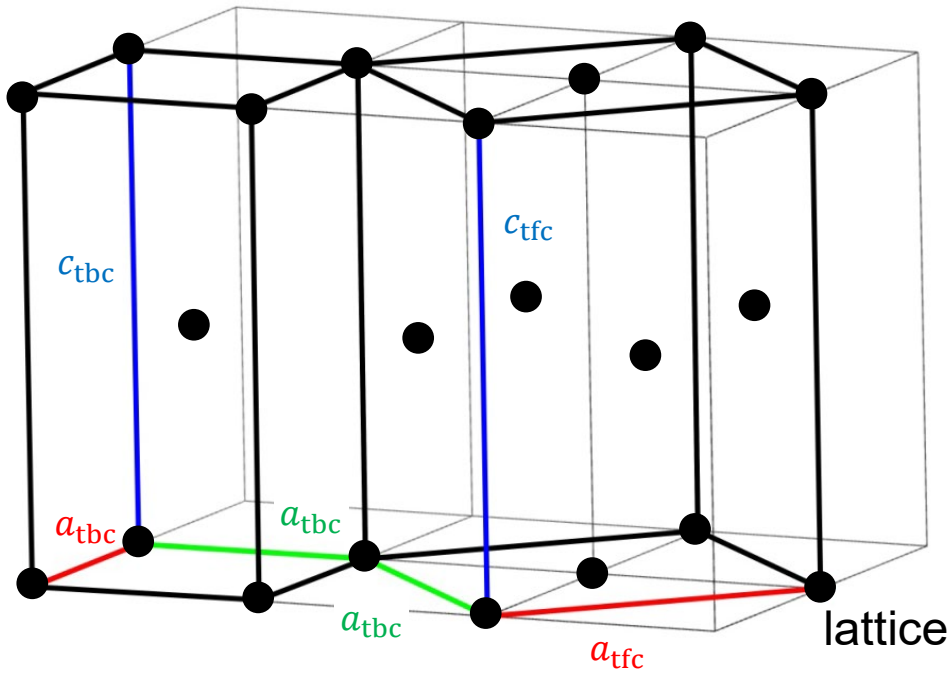
- Fourteen types of relevant point lattices **in crystallography with proper centering of the unit cell**. Relevant refers to the definition of the conventional cell. With centering, the cell is not primitive anymore.

Crystal System	Centering
triclinic	primitive
monoclinic	primitive and base-centered
orthorhombic	primitive, base-centered, body-centered and face-centered
tetragonal	primitive and body-centered
trigonal	primitive („rhombohedral“ = hex. cell with rhombohedral centering)
hexagonal	primitive
cubic	primitive, body-centered and face-centered



https://en.wikipedia.org/wiki/Crystal_system#Bravais_lattices

Example: tbc vs. tfc



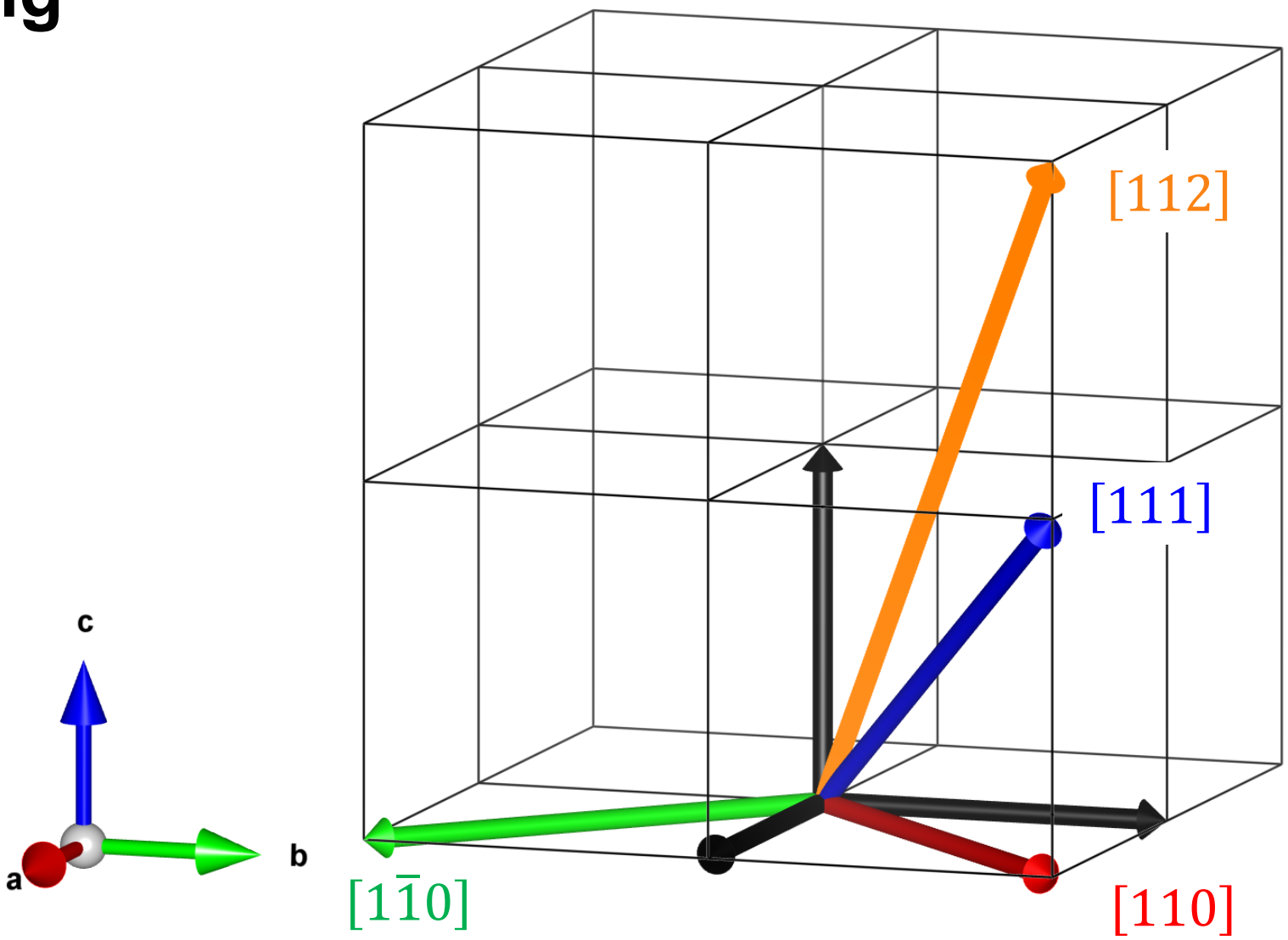
lattice points

Comparison of the equivalent descriptions of tbc and tfc (like for the Bain path in Fe-C martensites):

$$V_{\mathrm{tbc}} = a_{\mathrm{tbc}}^2\, c_{\mathrm{tbc}} < V_{\mathrm{tfc}} = a_{\mathrm{tfc}}^2\, c_{\mathrm{tfc}} = \left(\sqrt{2}a_{\mathrm{tbc}}\right)^2 \cdot c_{\mathrm{tbc}} = 2V_{\mathrm{tbc}}$$

The conventional cell in crystallography is always tbc, not tfc, since it has a smaller volume.

Indexing



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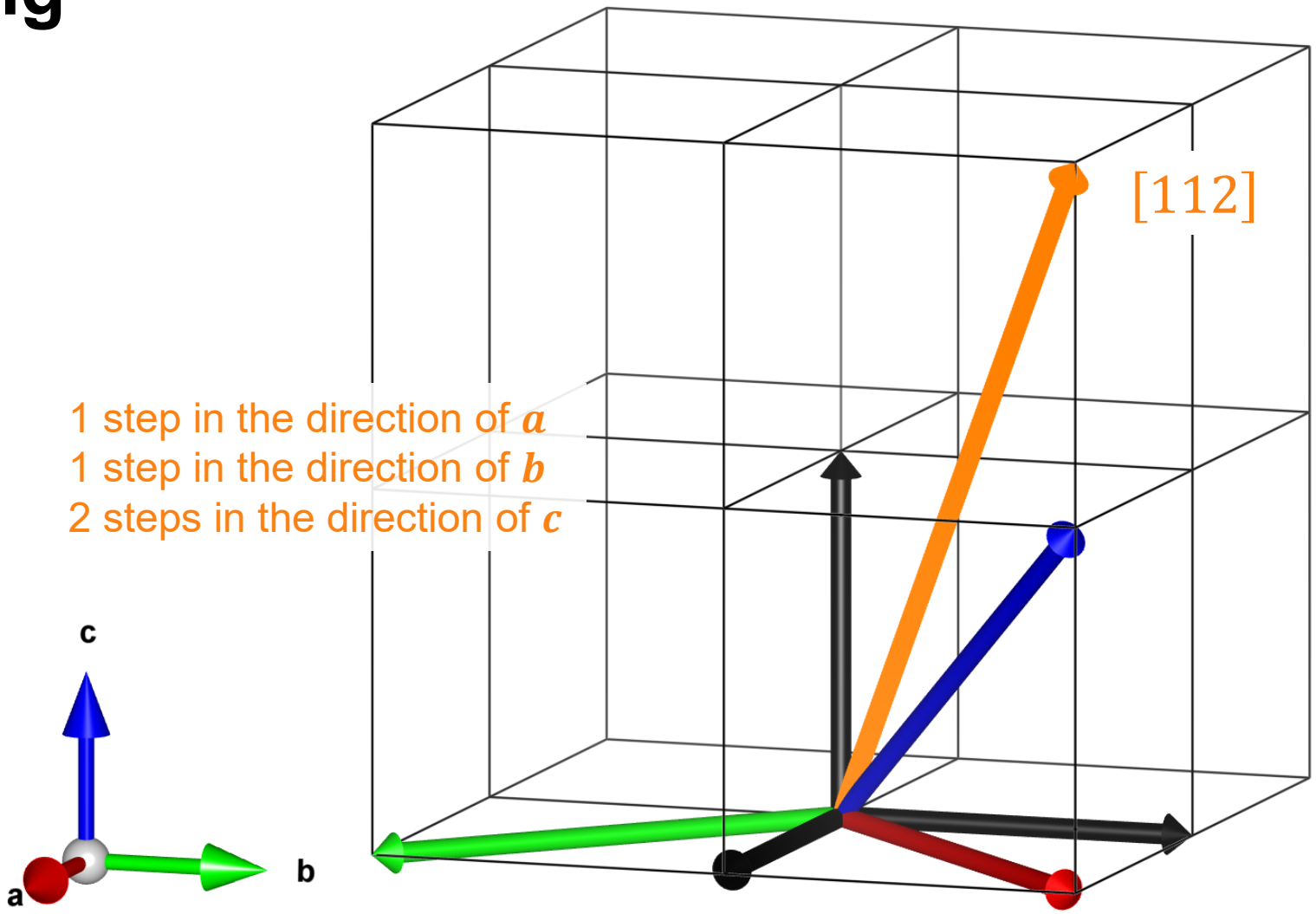

[112]
1 step in the direction of a
1 step in the direction of b
2 steps in the direction of c
c
a
b

Indexing

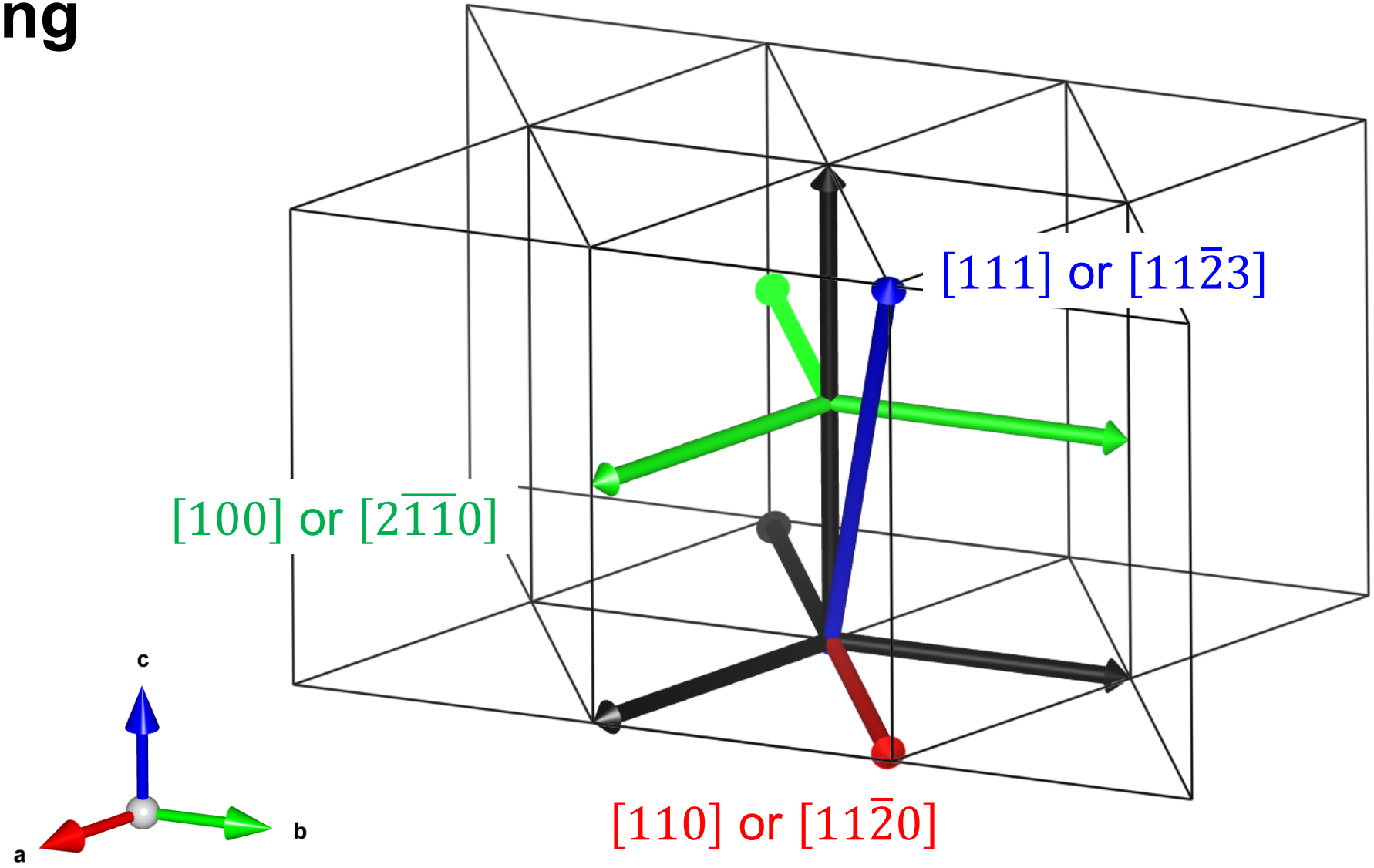
- Directions are indexed with respect to the axial basis of the unit cell.
- **Triplet indexing** of a direction $[uvw]$:

$$\boldsymbol{r} = u \cdot \boldsymbol{a} + v \cdot \boldsymbol{b} + w \cdot \boldsymbol{c}$$

- **Triplet indexing of direction families** $\langle uvw \rangle$ contains all crystallographic equivalent directions, like for example in a cubic crystal structure (all cube edges in this case):

$$\langle 001 \rangle = \begin{cases} [100] \\ [\bar{1}00] \\ [010] \\ [0\bar{1}0] \\ [001] \\ [00\bar{1}] \end{cases}$$

Indexing



Indexing

- Still the triplet indexing $[uvw]$ is valid:

$$\boldsymbol{r} = u \cdot \boldsymbol{a} + v \cdot \boldsymbol{b} + w \cdot \boldsymbol{c}$$

- There is an additional third vector in the basal plane which is crystallographic equivalent to first two: $\boldsymbol{a_1} = \boldsymbol{a}, \boldsymbol{a_2} = \boldsymbol{b}, \boldsymbol{a_3} = -\boldsymbol{a} - \boldsymbol{b}$
- Hence, quadruplet notation is possible $[u^* v^* t^* w^*]$ (Miller-Bravais):

$$\boldsymbol{r} = u^* \cdot \boldsymbol{a_1} + v^* \cdot \boldsymbol{a_2} + t^* \cdot \boldsymbol{a_3} + w^* \cdot \boldsymbol{c}$$

- The conversion follows:

$$u^* = \frac{(2u - v)}{3}$$

$$v^* = \frac{(2v - u)}{3}$$

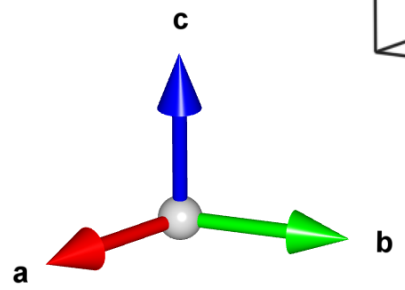
$$t^* = \frac{-(u + v)}{3}$$

$$w^* = w$$

Indexing

Triplet:
1 step in $\boldsymbol{a}$, 1 step in $\boldsymbol{b}$, none in $\boldsymbol{c}$, hence, $[110]$

Quadruplet:
conversion $u^* = \frac{(2\cdot1-1)}{3} = \frac{1}{3}, v^* = \frac{(2\cdot1-1)}{3} = \frac{1}{3}, t^* = \frac{-(1+1)}{3} = \frac{-2}{3}, w^* = 0$
co-prime indexing $[11\bar{2}0]$
(1 step in $\boldsymbol{a_1}$, 1 step in $\boldsymbol{a_2}$, 2 steps in $-\boldsymbol{a_3}$)



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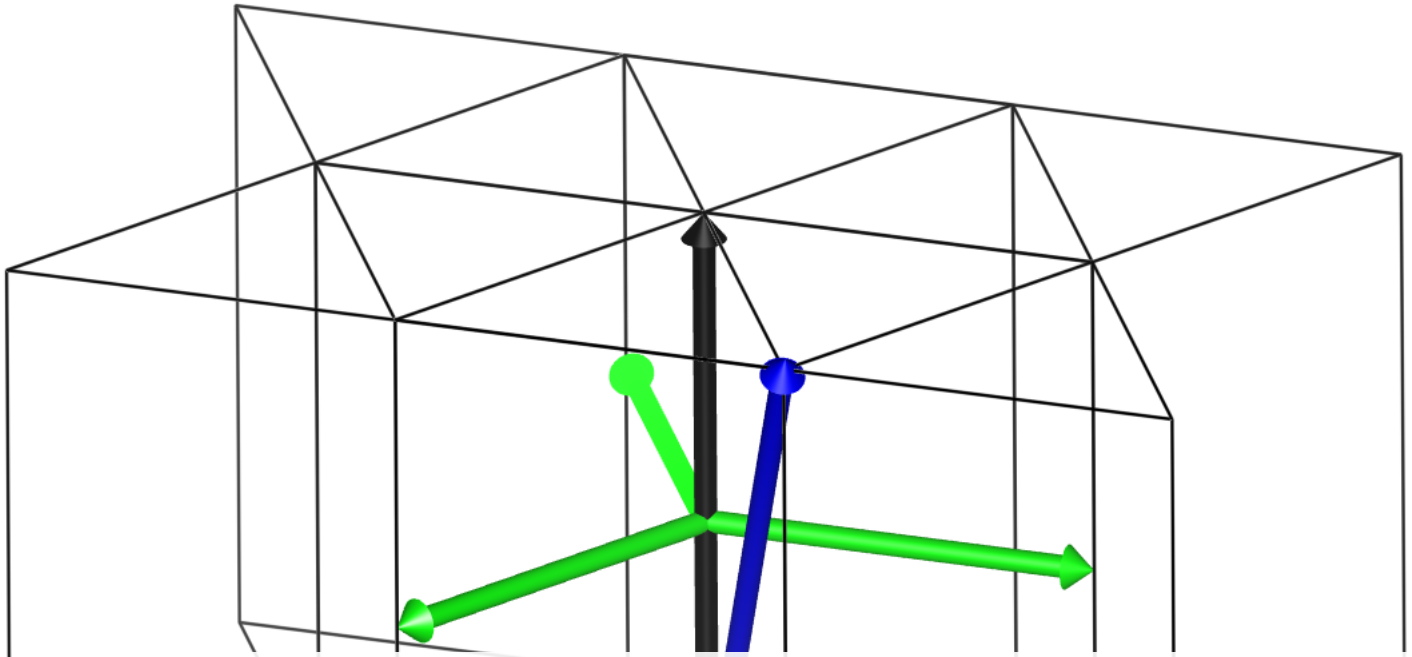
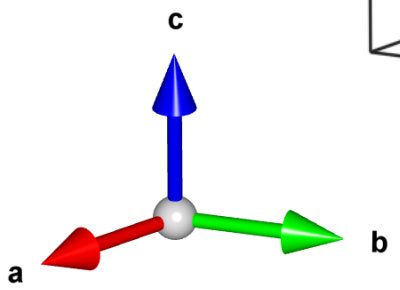




The quadruplet designation is used to easily identify crystallographic equivalent directions, for example within the basal plane:

$$[2\bar{1}\bar{1}0] \equiv [100]$$
$$[\bar{1}2\bar{1}0] \equiv [010]$$
$$[\bar{1}\bar{1}20] \equiv [\bar{1}\bar{1}0]$$

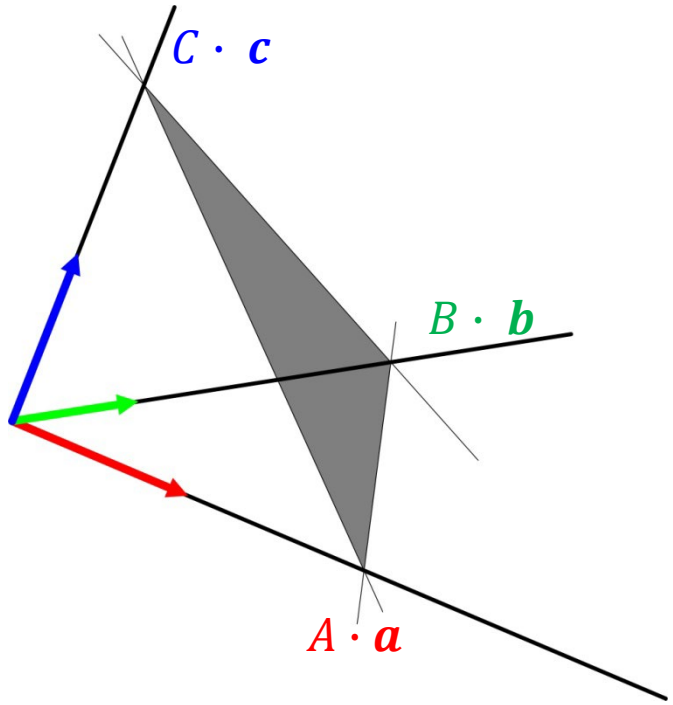
all belong to $\langle 100 \rangle$ (difficult to see) or better $\langle 11\bar{2}0 \rangle$.

Indexing

- Lattice planes are indexed with respect to the axial basis of the reciprocal lattice.
- **Triplet indexing** of a direction (hkl)
- Determination: determine the **intercepts of the plane with the axis of the (real) unit cell**, determine the **reciprocal numbers** (${}^{1}/_{\infty} = 0$), determine **co-prime indexing**
- Triplet indexing of a plane family $\{hkl\}$, contains all crystallographic equivalent directions, like for example for a cubic crystal structure (all cube facet in this case):

$$\{001\} = \begin{cases} (100) \\ (\bar{1}00) \\ (010) \\ (0\bar{1}0) \\ (001) \\ (00\bar{1}) \end{cases}$$

Reciprocal Lattice/Space



- Consider the intercepts of a plane with the basis axes to be: $A \cdot \boldsymbol{a}$, $B \cdot \boldsymbol{b}$, $C \cdot \boldsymbol{c}$.
- The **volume of the primitive cells** is then (area of the plane multiplied by the normal vector $\boldsymbol{n}$ of the plane as the height of the primitive cell):
- $V = \big((B\,\boldsymbol{b} - C\,\boldsymbol{c}\,) \times (A\,\boldsymbol{a} - C\,\boldsymbol{c})\big) \cdot \boldsymbol{n}$

$$V = (AB\,\boldsymbol{a} \times \boldsymbol{b} - AC\,\boldsymbol{a} \times \boldsymbol{c} - BC\,\boldsymbol{c} \times \boldsymbol{b} + CC\,\boldsymbol{c} \times \boldsymbol{c}) \cdot \boldsymbol{n}$$

- with $\boldsymbol{c} \times \boldsymbol{c} = \boldsymbol{0}$:

$$V = (AB\,\boldsymbol{a} \times \boldsymbol{b} + AC\,\boldsymbol{c} \times \boldsymbol{a} + BC\,\boldsymbol{b} \times \boldsymbol{c}) \cdot \boldsymbol{n}$$

- and $BC = h, AC = k, BC = l$:

$$V = (h\,\boldsymbol{a} \times \boldsymbol{b} + k\,\boldsymbol{c} \times \boldsymbol{a} + l\,\boldsymbol{b} \times \boldsymbol{c}) \cdot \boldsymbol{n}$$

- The volume can be described by three alternative basis vectors:
  - $\boldsymbol{a}' = \frac{2\pi}{V}\boldsymbol{a} \times \boldsymbol{b}, \quad \boldsymbol{b}' = \frac{2\pi}{V}\boldsymbol{c} \times \boldsymbol{a}, \quad \boldsymbol{c}' = \frac{2\pi}{V}\boldsymbol{b} \times \boldsymbol{c}$
- These vector are the basis of the reciprocal lattice; note the $1/\mathrm{m}$ unit of the axes.

Reciprocal Lattice/Space

- The basis vectors are $\boldsymbol{a'} = \frac{2\pi}{V}\boldsymbol{b} \times \boldsymbol{c}$, $\boldsymbol{b'} = \frac{2\pi}{V}\boldsymbol{c} \times \boldsymbol{a}$, $\boldsymbol{c'} = \frac{2\pi}{V}\boldsymbol{b} \times \boldsymbol{a}$.
  In solid state physics, the 2π factor is often used due to easier description of wave and diffraction phenomena. In crystallography, the 2π factor is often omitted.
- Every rational vector of the reciprocal space $\boldsymbol{G} = h\boldsymbol{a'} + k\boldsymbol{b'} + l\boldsymbol{c'}$ is **always perpendicular to the set of parallel lattice planes** given by the **Miller triplet** (hkl). Its **length** corresponds to the **reciprocal distance of the lattice planes**: $d_{hkl} = \frac{2\pi}{|\boldsymbol{G}|}$.
- **Diffraction** occurs when (Laue condition) the wave vector difference between incident and diffracted beam is equal to a reciprocal vector: $\Delta\boldsymbol{k} = \boldsymbol{G}$.

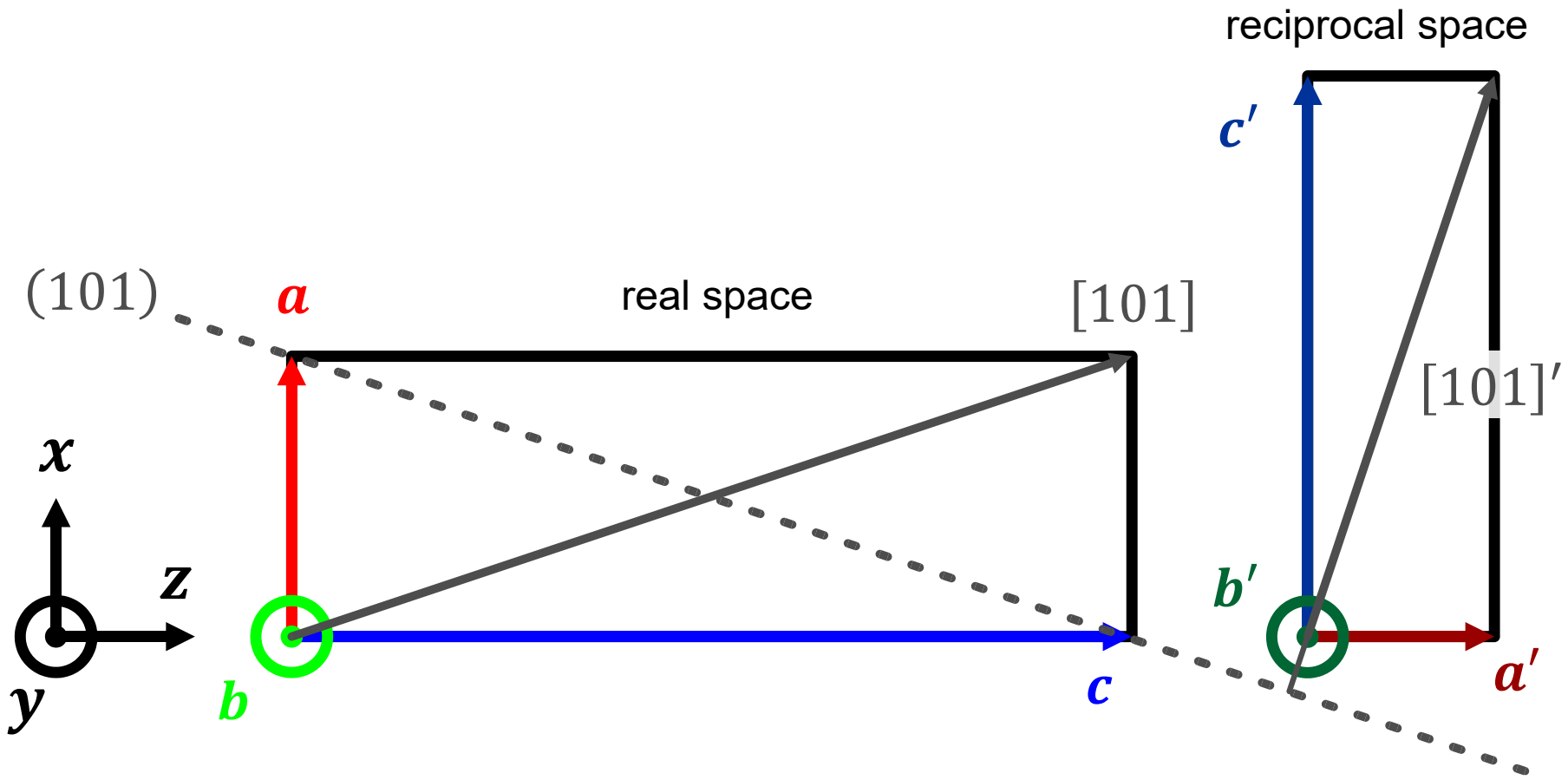
Reciprocal Lattice/Space

- Cartesian reference system: $\boldsymbol{x}$, $\boldsymbol{y}$, $\boldsymbol{z}$ are perpendicular to each other and are unit vectors.
- A tetragonal crystal system is built up from: $\boldsymbol{a} = a\,\boldsymbol{x}, \boldsymbol{b} = a\,\boldsymbol{y}, \boldsymbol{c} = c\,\boldsymbol{z}$
- The volume of the unit cell is then: $V = (\boldsymbol{a} \times \boldsymbol{b}) \cdot \boldsymbol{c} = a^2\,c$
- The basis vectors of the reciprocal space are:

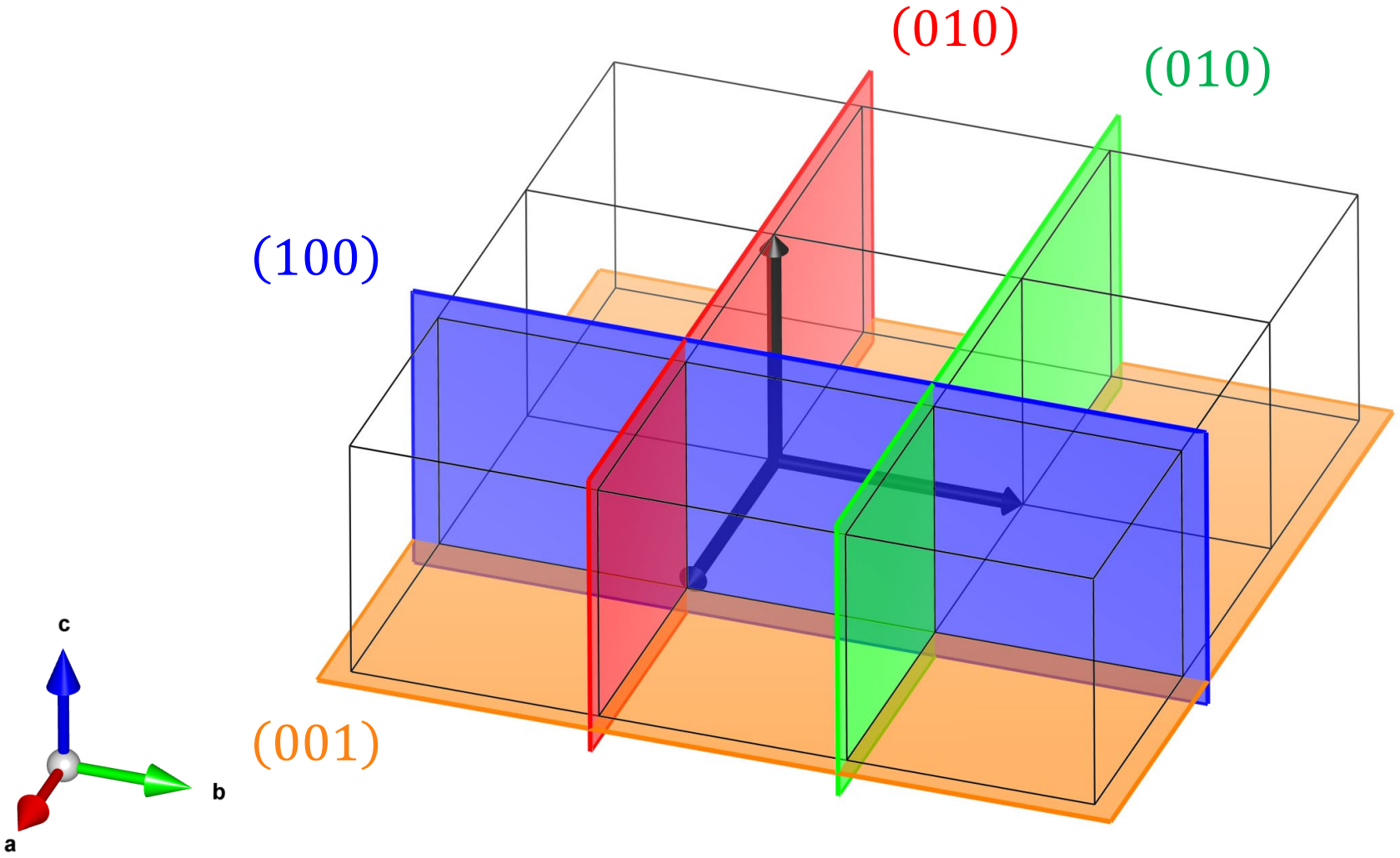
$$\boldsymbol{a}' = \frac{2\pi}{c}\boldsymbol{z}, \boldsymbol{b}' = \frac{2\pi}{a}\boldsymbol{y}, \boldsymbol{c}' = \frac{2\pi}{a}\boldsymbol{x}$$

- The crystallographic direction $[101]$ lies along the vector $a\,\boldsymbol{x} + c\,\boldsymbol{z}$ which is $\begin{pmatrix} a \\ 0 \\ c \end{pmatrix}$ in the cartesian reference system.
- Though, the plane normal of (101) is along the reciprocal lattice vector, namely $\frac{2\pi}{c}\boldsymbol{z} + \frac{2\pi}{a}\boldsymbol{x}$, which is $2\pi\begin{pmatrix} 1/a \\ 0 \\ 1/c \end{pmatrix}$ in the Cartesian reference.
- **In all non-cubic crystal systems, the crystallographic direction $[hkl]$ given for a set of lattice planes (hkl) is not parallel to the respective plane normal!**

Reciprocal Lattice/Space



Indexing



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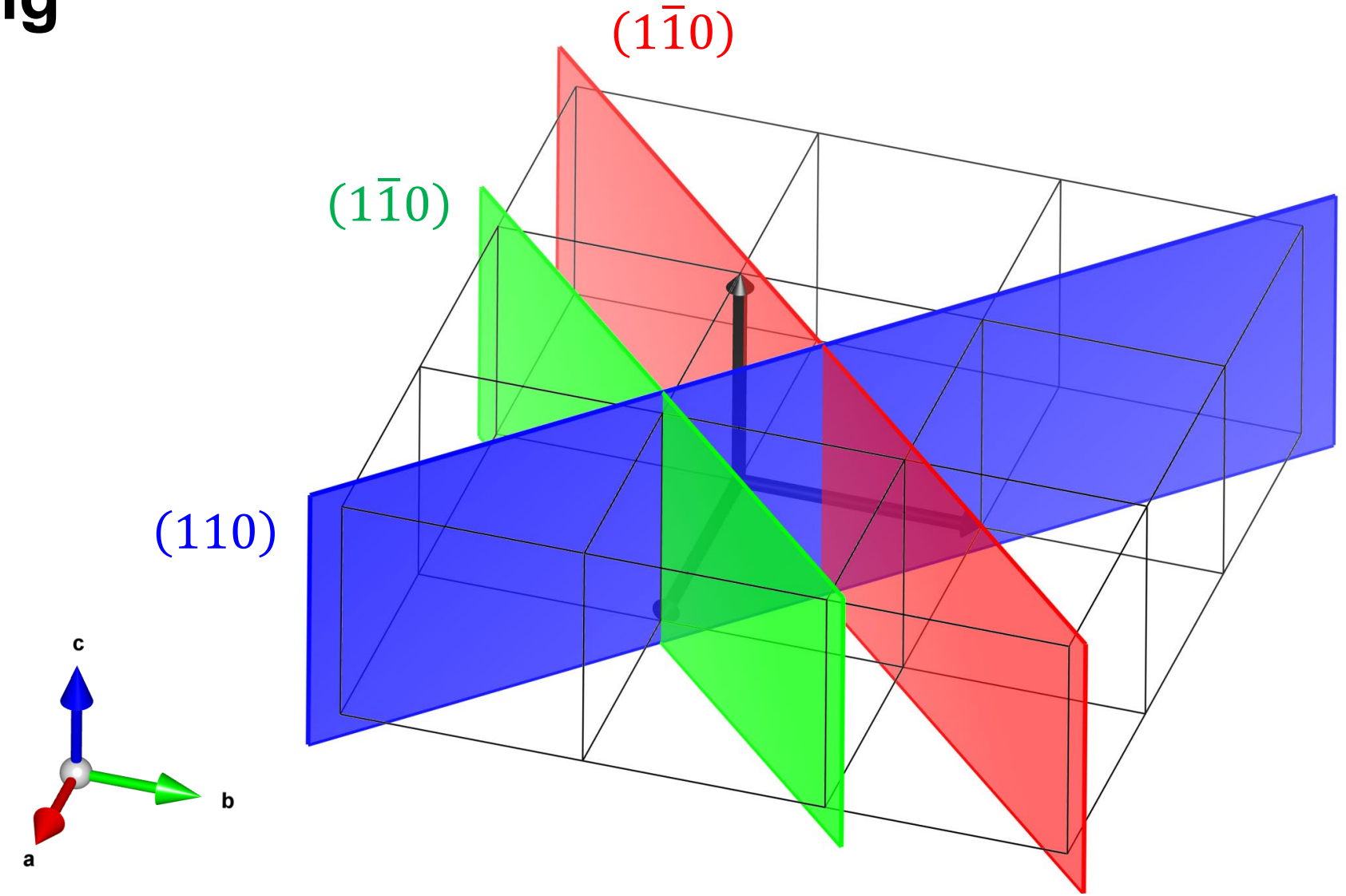

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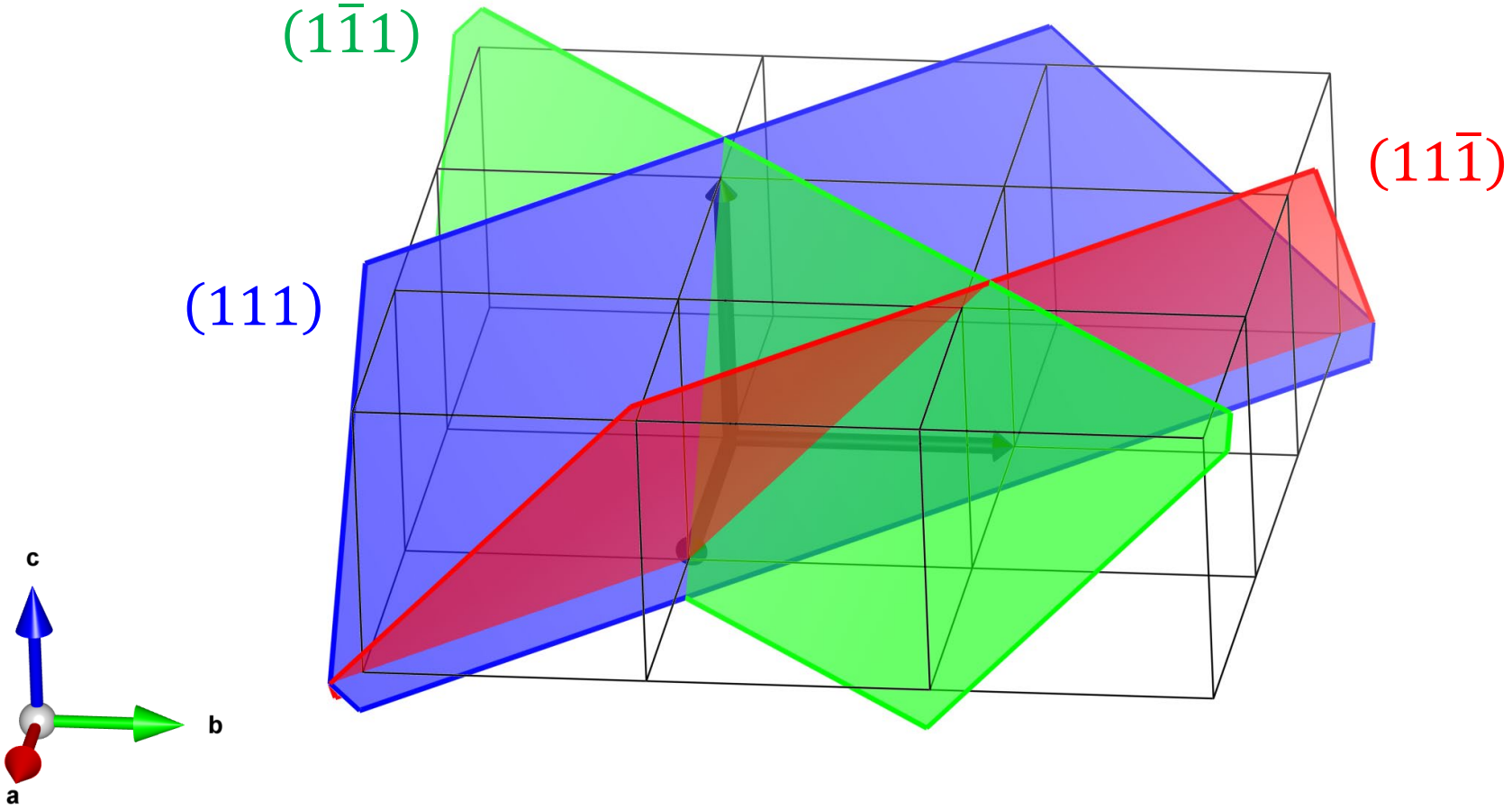
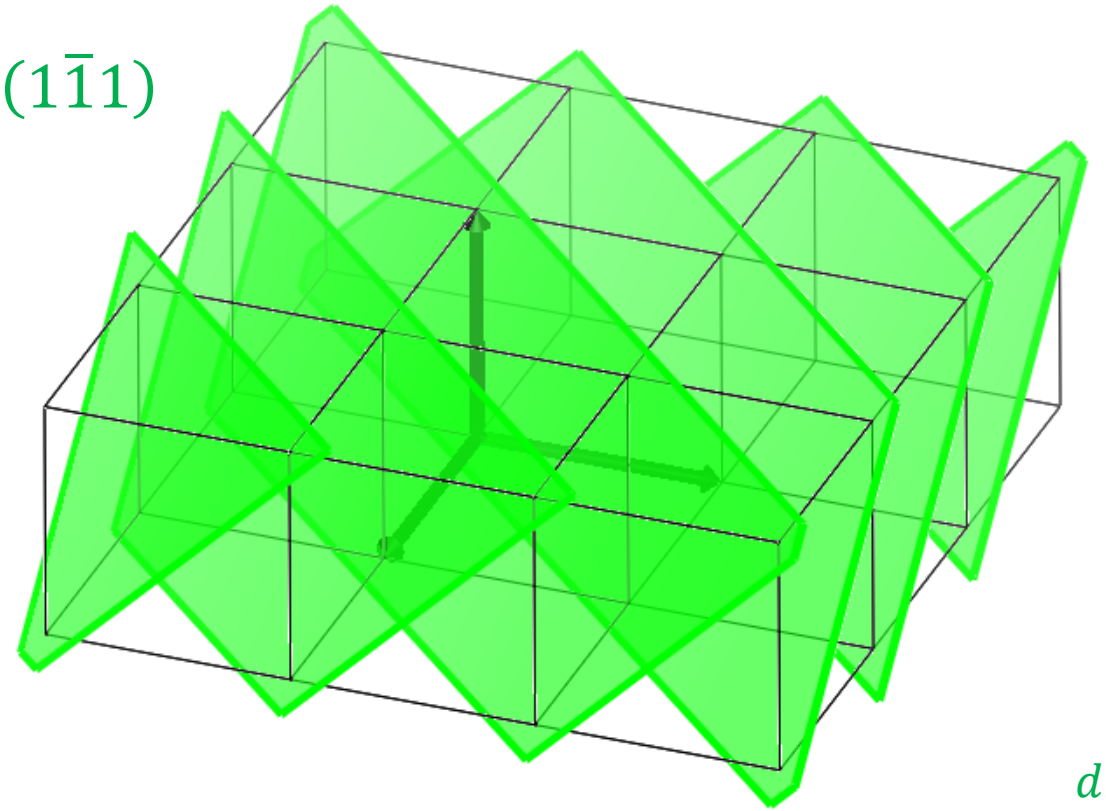


Indexing

Attention: A Miller triplet always describes the entire set of parallel lattice planes, not a single plane!

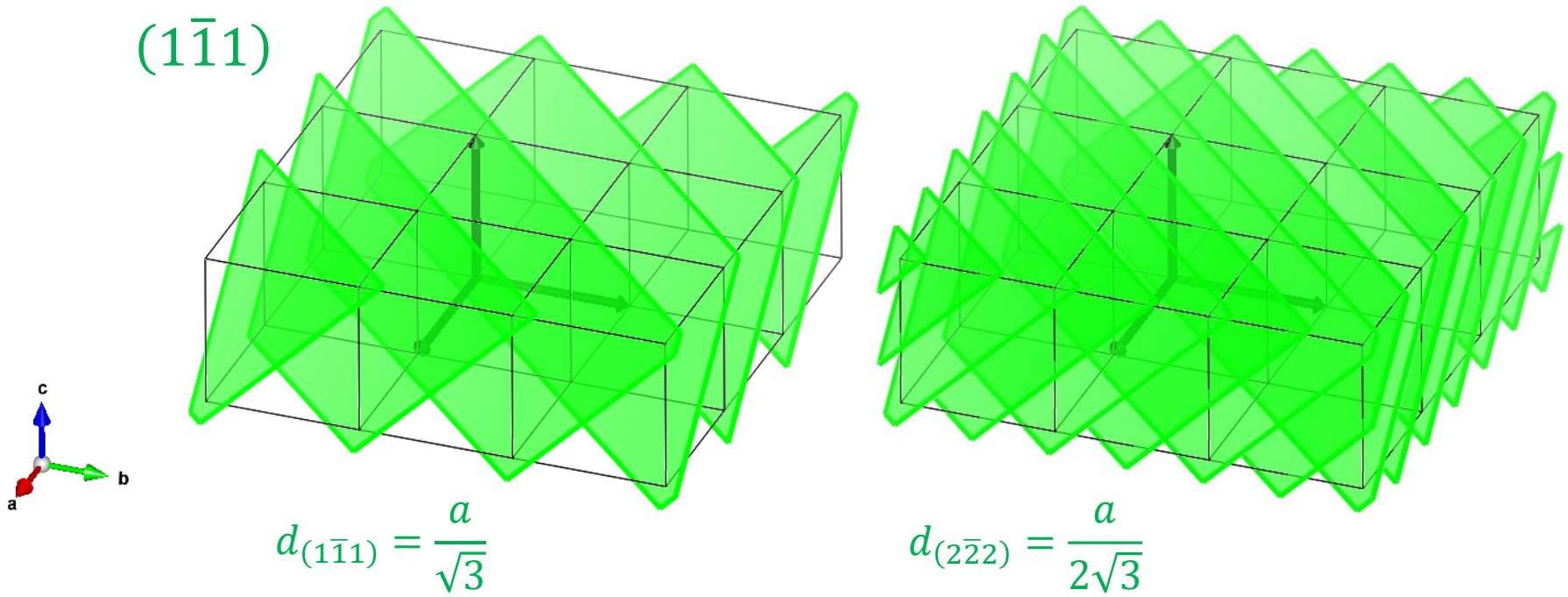
$(1\bar{1}1)$



$$d_{(1\bar{1}1)} = \frac{a}{\sqrt{3}}$$

Indexing

- **Miller indices should be co-prime.** In literature, **Laue indices** are often used instead which also include higher order indices. These indicate different spacing between the planes (the direction of $\boldsymbol{G}$ remains the same but its length becomes larger; corresponds to smaller spacing).

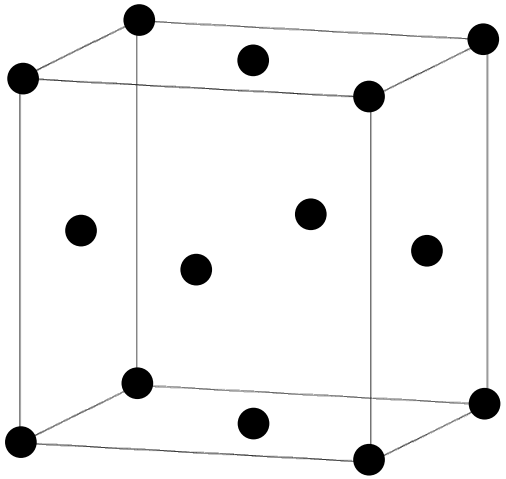


Common Short Notations: Prototype

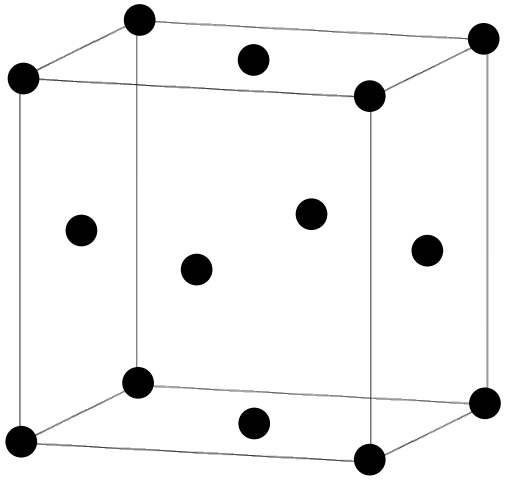
- Structures of the same structure type possess the same symmetry and the same occupation of lattice sites. All structure types are called according to a prototype phase.
- For example Cu structure type:
  - **Most of the face-centered cubic metals**
  - Information from the designation as “Cu structure type” is: space group no. 225 (symmetry information), a single element on the Wyckoff position *4a* (lattice site information)
  - Additional information necessary to built up the crystal: lattice parameter and type of the atom being placed on the lattice site
- for example diamond structure type:
  - **All face-centered cubic, elemental semiconductors**
  - Information from the designation as “diamond structure type” is: space group no. 227 (symmetry information), a single element on the Wyckoff position *8a* (lattice site information)

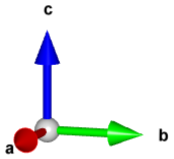
Common Short Notations: Prototype

fcc



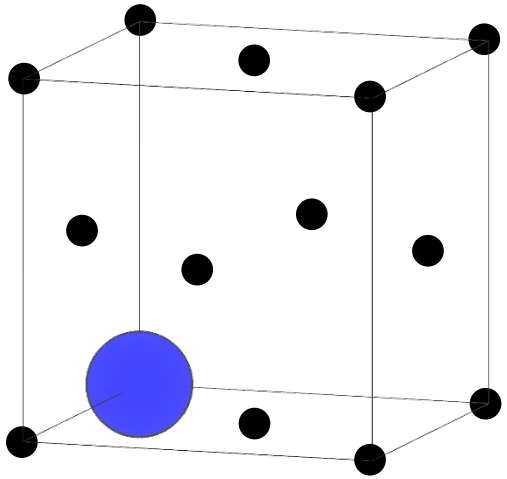
fcc



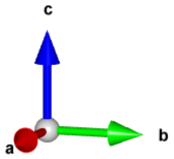


Common Short Notations: Prototype

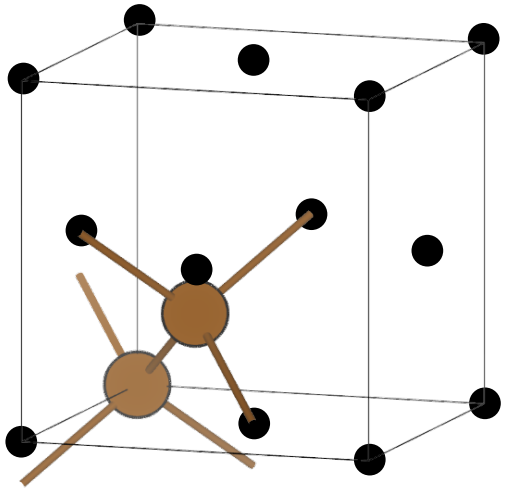
Cu

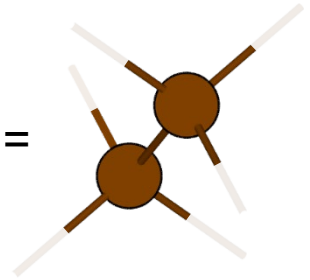


Basis: ● = 



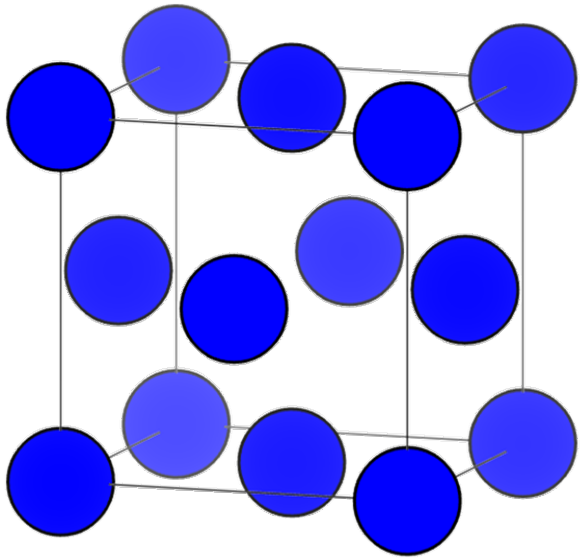
diamond



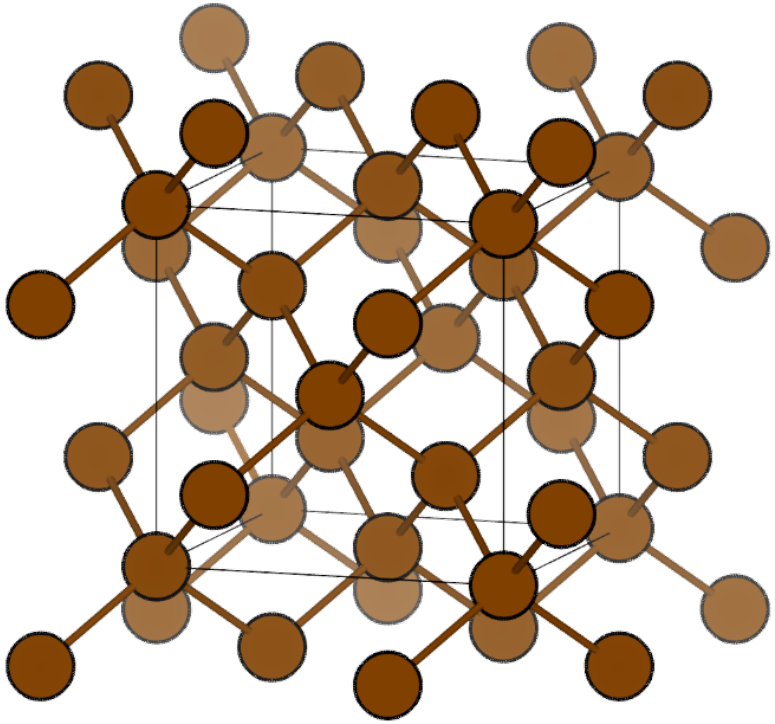
Basis: ● = 

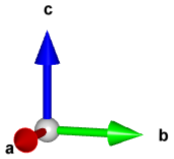
Common Short Notations: Prototype

Cu



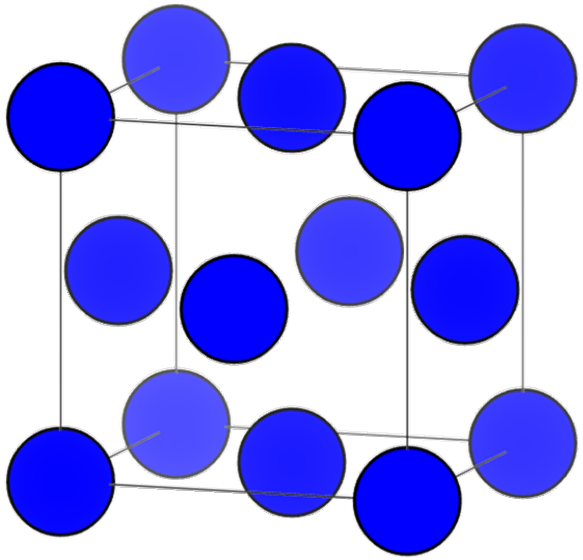
diamond



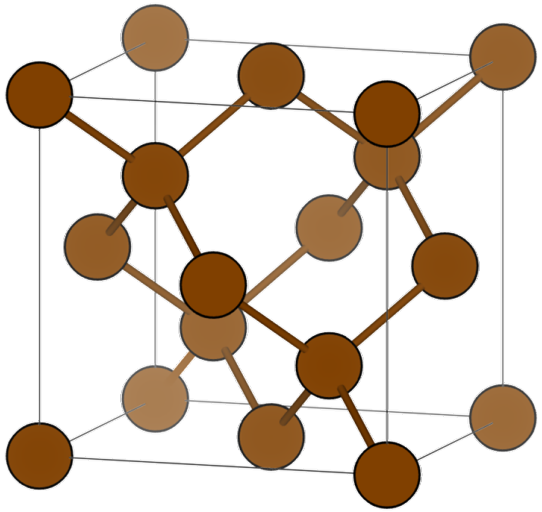


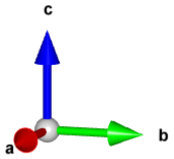
Common Short Notations: Prototype

Cu



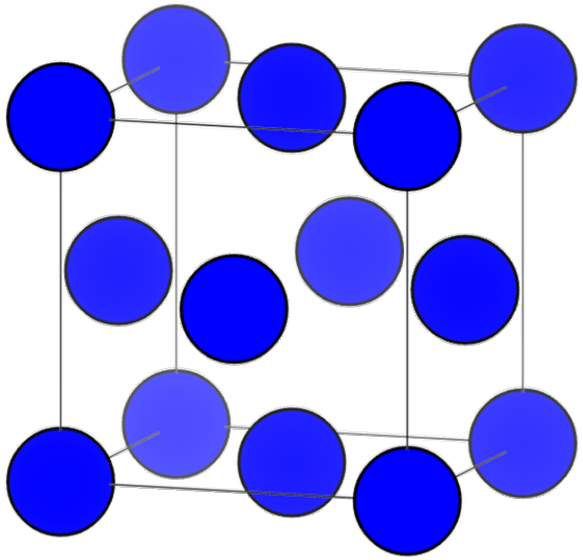
diamond



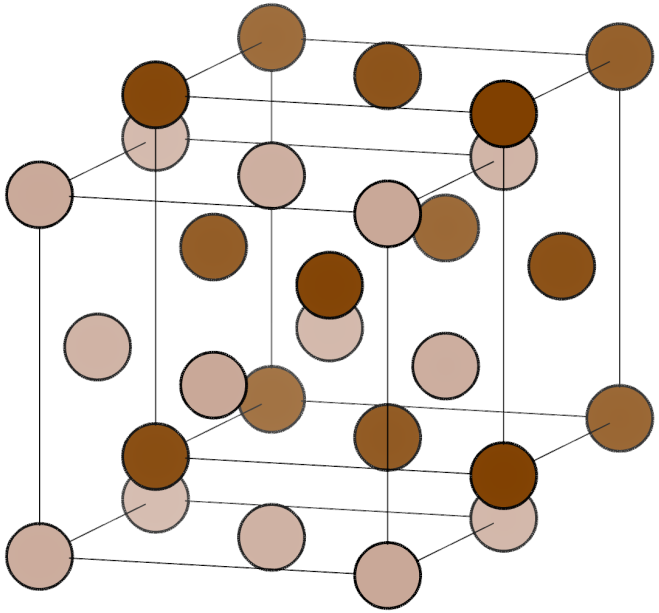


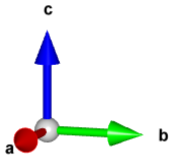
Common Short Notations: Prototype

Cu



diamond





Common Short Notations: Strukturbericht

- Set of short notation based on the following groups and the respective observation of prototype materials:

Designation	Type of element/alloy/compound
A	elements
B	compounds AB
C	compounds AB_2
D	simple compounds A_mB_n
E … K	complex compounds
L	alloys
O	organics
S	silicates

http://www.geocities.jp/ohba_lab_ob_page/Structure.html

Common Short Notations: Strukturbericht

Designation	Prototype
A1	**Cu**
A2	**W**
A3	**Mg**
A4	**Diamond**
A5	β-Sn
A6	In
A7	As
A8	γ-Se
A9	Graphite
A12	**α-Mn**
A13	β-Mn
A14	I_2
A15	**Cr_3Si**
A_h	α-Po

…

Wrongly assigned to elements as first expected to be a modification of W but later identified as WO_3.

http://www.geocities.jp/ohba_lab_ob_page/Structure.html

Common Short Notations: Strukturbericht

Designation	Prototype
B1	NaCl
B2	**CsCl**
B3	Sphalerite ZnS
B4	Wurtzite ZnS

...

http://www.geocities.jp/ohba_lab_ob_page/Structure.html

Common Short Notations: Strukturbericht

Designation	Prototype
C1	Fluorite CaF_2
C2	Pyrite FeS_2
C3	Cuprite Cu_2O
C4	**Rutile TiO_2**
C5	**Anatase TiO_2**
C8	**β-Quartz SiO_2**
C8a	**α-Quartz SiO_2**
C9	**Cristobalite SiO_2**
C10	**Tridymite SiO_2**
C14	**$MgZn_2$ hex. Laves phase**
C15	**Cu_2Mg kub. Laves phase**
C21	**Brookite TiO_2**
C36	**$MgNi_2$ hex. Laves phase**

...

http://www.geocities.jp/ohba_lab_ob_page/Structure.html

Common Short Notations: Strukturbericht

Designation	Prototype
$D0_2$	Skutterudite $CoAs_3$
$D0_{11}$	**Cementite Fe_3C**
$D5_1$	**Corundum Al_2O_3**
$E2_1$	(ideal) Perovskite $CaTiO_3$
$G0_1$	Calcite $CaCO_3$
$G0_2$	Aragonite $CaCO_3$
$H1_1$	**Spinell $MgAl_2O_4$**
$L1_1$	**AuCu**
$L1_2$	**Cu_3Au**
$L2_1$	**Cu_2AlMn Heusler phase**

...

http://www.geocities.jp/ohba_lab_ob_page/Structure.html

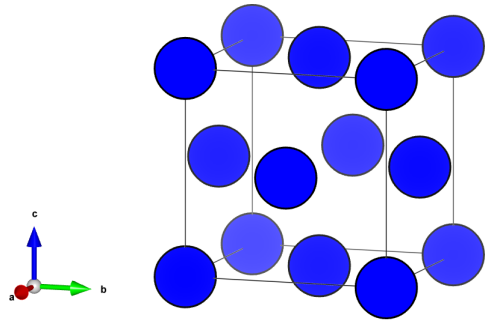
Common Structures of Metals

- **Metallic binding is omnidirectional**. Hence, **similar principles of structure formation** are found for most metallic materials: **the crystal structures are of high coordination**; maximum number of nearest neighbors and packing density is achieved.
- There are only few different crystal structures observed among metallic materials:

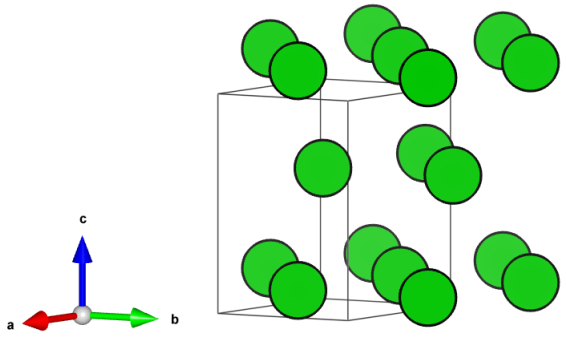
Prototype	Strukturbericht	Examples
Cu	**A1**	Cu, Al, Au, Ni, Ag, β-Co, γ-Fe, etc.
W	**A2**	W, Cr, α-Fe, Na, K, Nb, Cr, β-Ti, etc.
Mg	**A3**	Mg, α-Ti, Zn, α-Co, etc.

- Exceptions are arising from the appearance of different types of magnetic coupling or contributions from other types of atomic binding. For example, bcc α-Mn with 58 atoms in the unit cell, or sc α-Po.

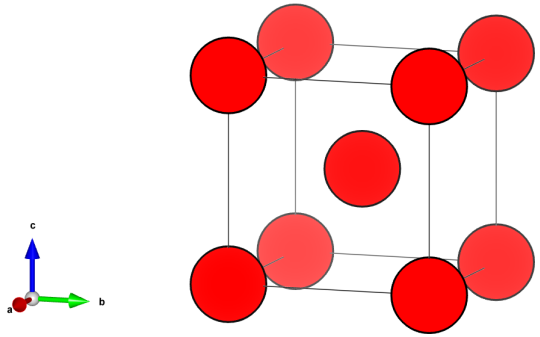
Common Structures of Metals



Cu
coordination: 12
no. of atoms in the unit cell: 4
atomic packing factor: 74 %
closed packed directions: $\langle 110 \rangle$
closed packed planes: $\{111\}$

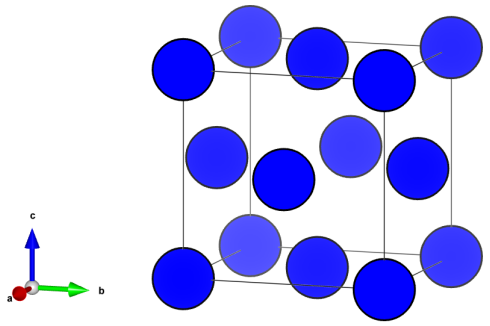


Mg
coordination: 12
no. of atoms in the unit cell: 2
atomic packing factor: 74 %
closed packed directions: $\langle 11\bar{2}0 \rangle$
closed packed planes: $\{0001\}$



W
coordination: 8
no. of atoms in the unit cell: 2
atomic packing factor: 68 %
close packed directions: $\langle 111 \rangle$
***densely* packed planes:** $\{110\}$

Properties



Cu

coordination: $12 = 6 + 3 + 3$

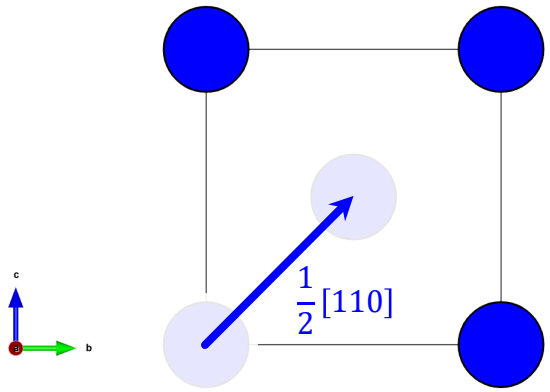
(within the plane, above the plane, and below the plane)

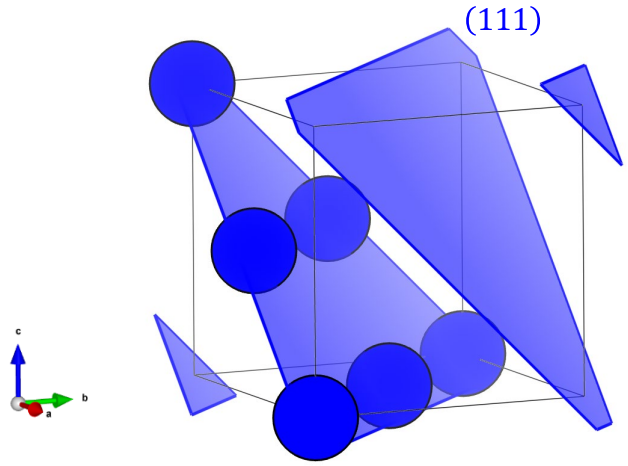
no. of atoms in the unit cell: $6 \cdot \frac{1}{2} + 8 \cdot \frac{1}{8} = 4$

atomic packing factor: $74\ \%$

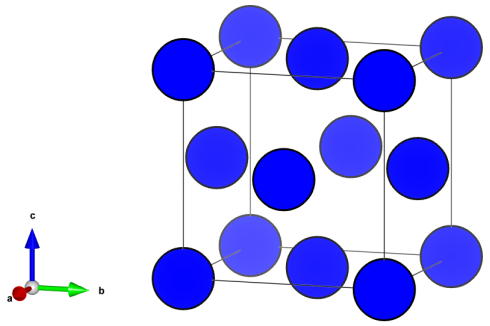
closed packed directions: $\langle 110 \rangle$

closed packed planes: $\{111\}$





Properties



Cu

coordination: $12 = 6 + 3 + 3$

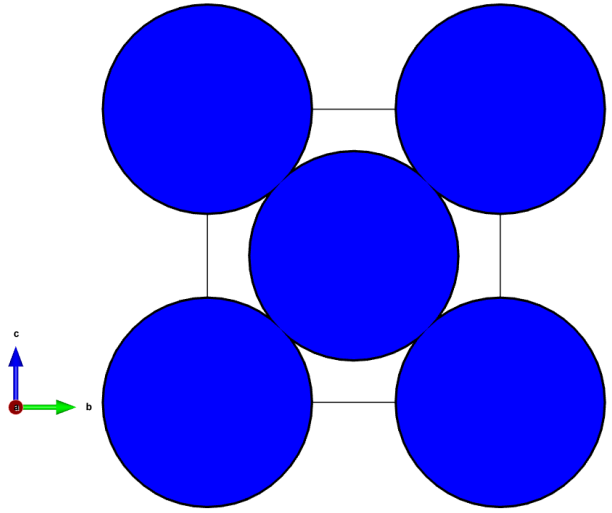
(within the plane, above the plane, and below the plane)

no. of atoms in the unit cell: $6 \cdot \frac{1}{2} + 8 \cdot \frac{1}{8} = 4$

atomic packing factor: $74\ \%$

closed packed directions: $\langle 110 \rangle$

closed packed planes: $\{111\}$

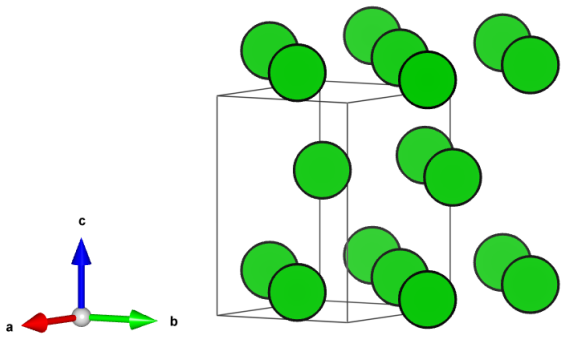


$$PF = \frac{N_\mathrm{a} \cdot V_\mathrm{a}}{V_\mathrm{uc}} = \frac{4 \cdot \frac{4}{3}\pi R^3}{a^3}$$

$$4R = \sqrt{2}a$$

$$PF = \frac{\sqrt{2}}{6}\pi$$

Properties



Note that the crystallographic description of hcp is slightly different from almost all textbook descriptions. The Wyckoff position 2c is not placed in the origin of the unit cell.

Mg

coordination: $12 = 6 + 3 + 3$
(within the plane, above the plane, and below the plane)

no. of atoms in the unit cell:

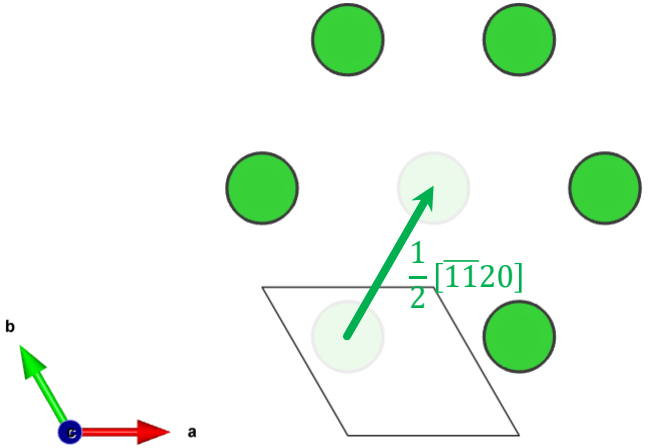
$2 \cdot 1 = 2$ (crystallographic version)

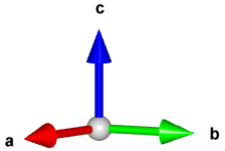
$4 \cdot \frac{1}{12} + 4 \cdot \frac{1}{6} + 1 \cdot \frac{2}{3} + 1 \cdot \frac{1}{3} = 2$ (in the version of most textbooks)

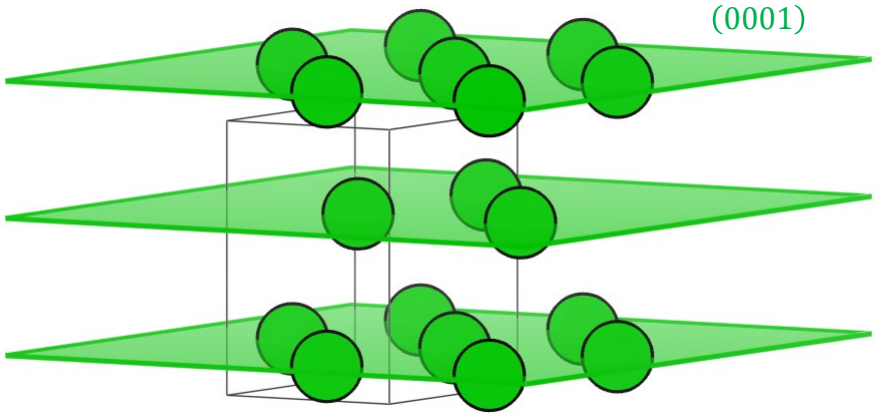
atomic packing factor: $74\ \%$

closed packed directions: $\langle 11\bar{2}0 \rangle$

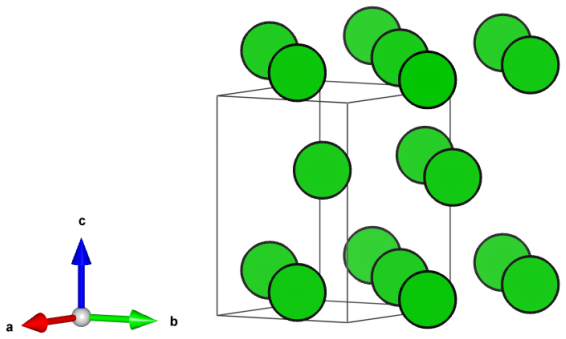
closed packed planes: $\{0001\}$



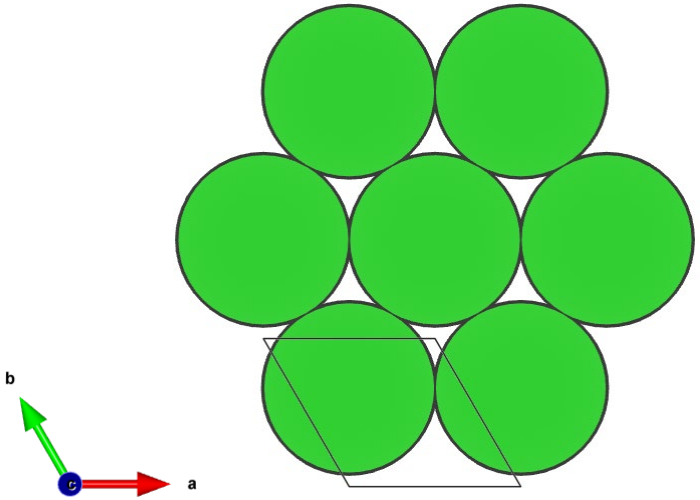




Properties



Mg
coordination: 12
no. of atoms in the unit cell: 2
atomic packing factor: 74 %
closed packed directions: $\langle 11\bar{2}0 \rangle$
closed packed planes: $\{0001\}$



$$PF = \frac{N_\mathrm{a} \cdot V_\mathrm{a}}{V_\mathrm{uc}} = \frac{2 \cdot \frac{4}{3}\pi R^3}{a^2\, c \sin 60°}$$

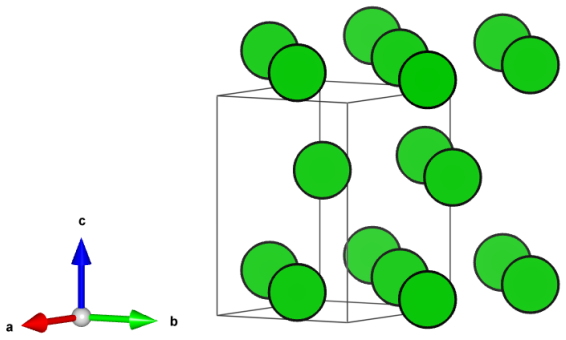
$$2R = a$$

$$PF = \frac{2\sqrt{3}}{9}\pi\frac{a}{c}$$

$$\left.\frac{c}{a}\right|_\mathrm{ideal} = \sqrt{\frac{8}{3}}$$

$$\left.PF\right|_\mathrm{ideal} = \frac{2}{3\sqrt{8}}\pi$$

Properties



Mg
coordination: 12
no. of atoms in the unit cell: 2
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closed packed directions: $\langle 11\bar{2}0 \rangle$
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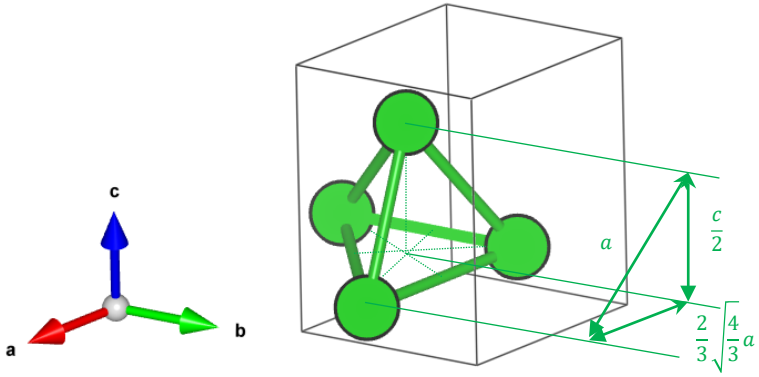
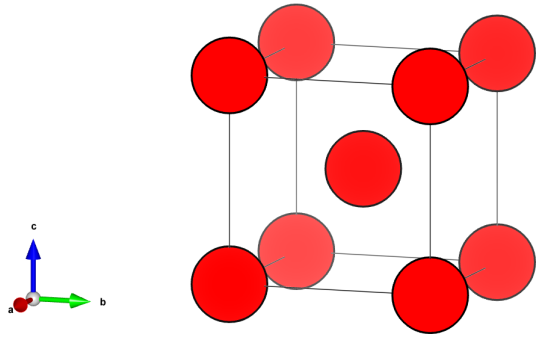


The atoms form regular triangles of a in length. The height is $\sqrt{\frac{4}{3}}a$. The distance to the next plane always corresponds to $\frac{c}{2}$.
In case of ideal packing, the atoms from the plane above also exhibit a nearest neighbor distance of a and the atom is exactly placed in the void at $\frac{2}{3}$ of the height of the regular triangles:

$$\frac{c}{2} = \sqrt{a^2 - \left(\frac{1}{2}\sqrt{\frac{4}{3}}a\right)^2} = \sqrt{\frac{2}{3}}a$$

$$\frac{c}{a} = \sqrt{\frac{8}{3}}$$

Properties



W

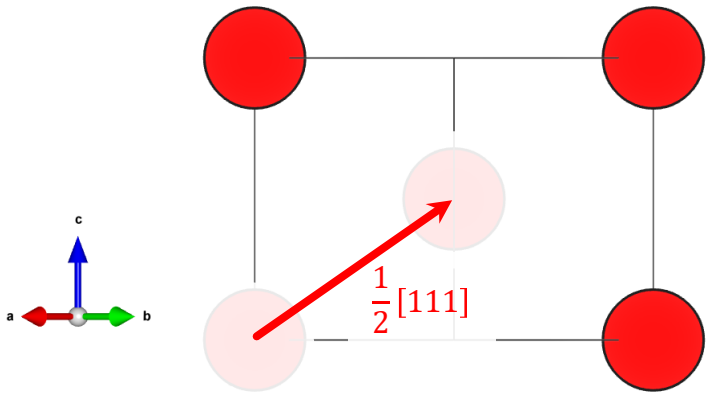
coordination: 8

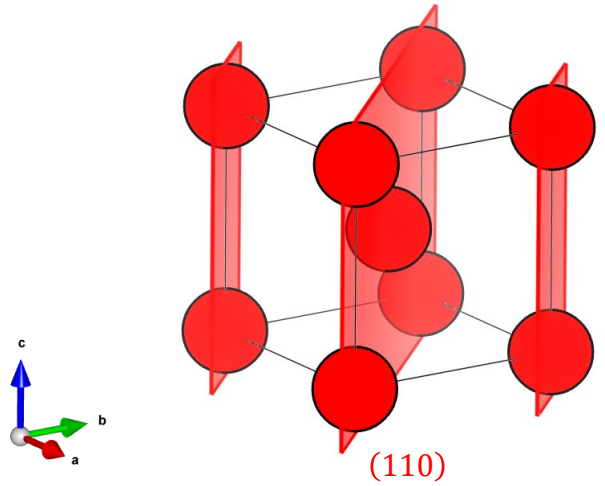
no. of atoms in the unit cell: $1 \cdot 1 + 8 \cdot \frac{1}{8} = 2$

atomic packing factor: 68 %

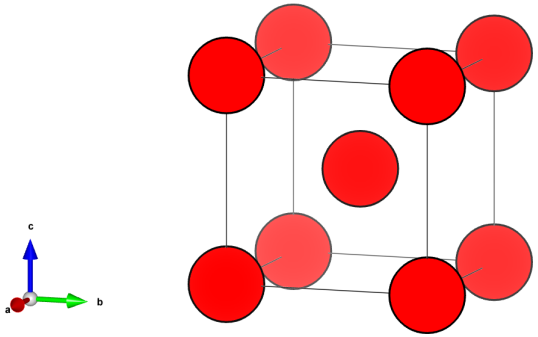
close packed directions: $\langle 111 \rangle$

***densely* packed planes:** $\{110\}$





Properties



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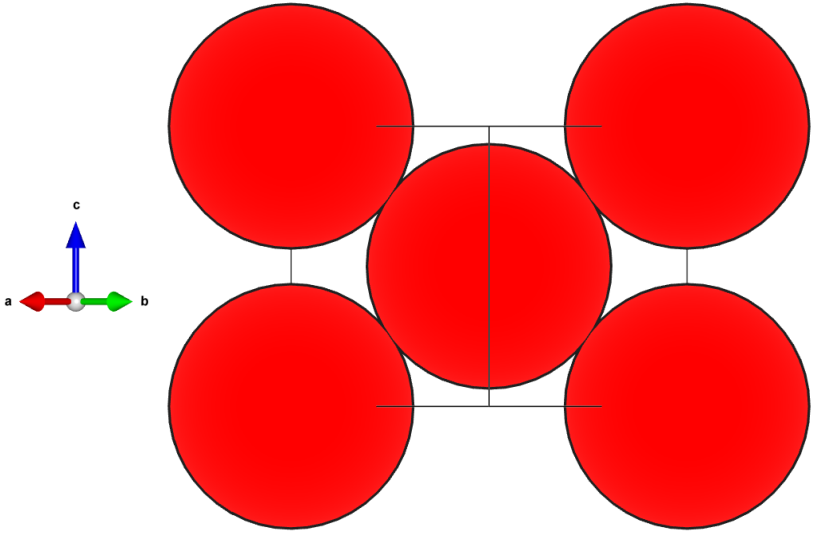


$$PF = \frac{N_\mathrm{a} \cdot V_\mathrm{a}}{V_\mathrm{uc}} = \frac{2 \cdot \frac{4}{3}\pi R^3}{a^3}$$

$$4R = \sqrt{3}a$$

$$PF = \frac{\sqrt{3}}{8}\pi$$

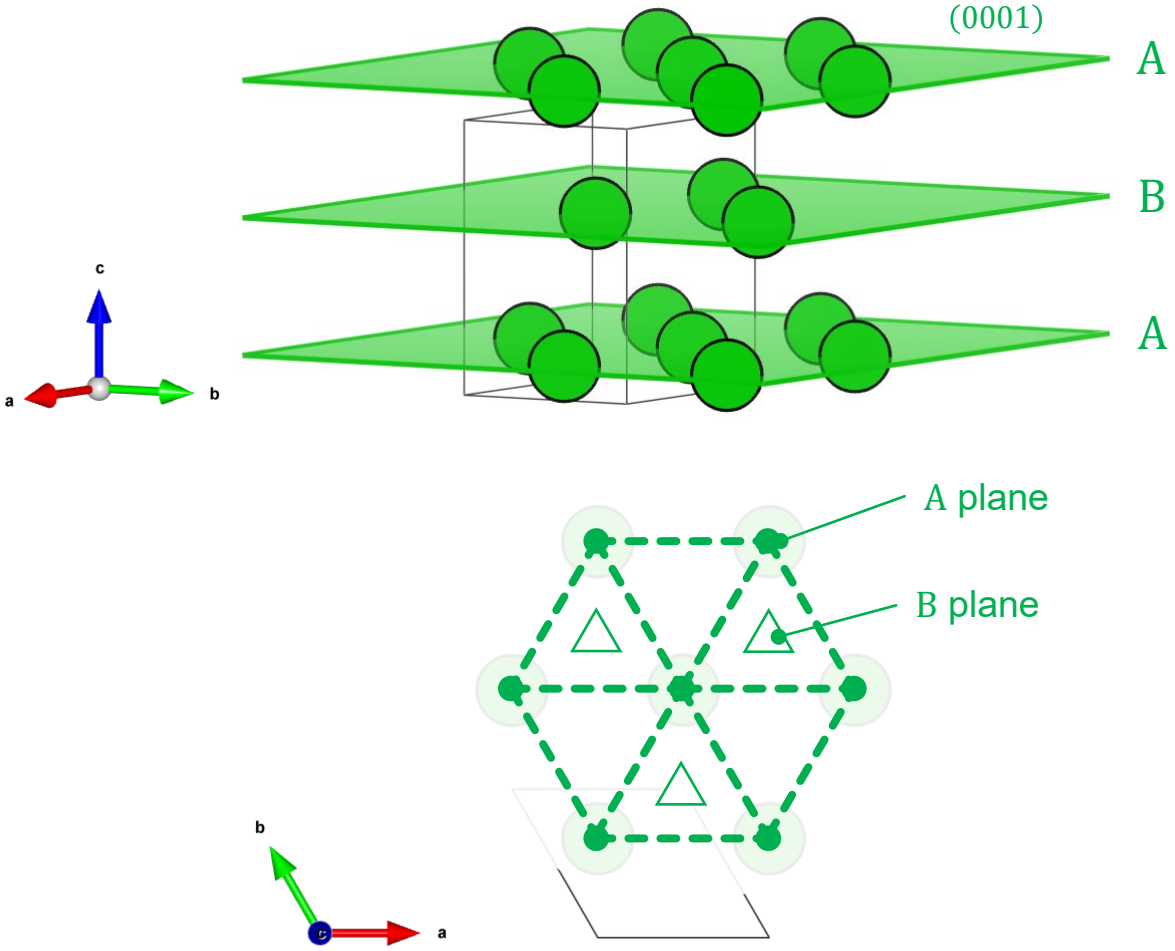
Closed-Packed Structures

- The question for closed packed structures of rigid spheres goes back to Johannes Kepler in 1611. He was not able to find a prove for his conjecture that there is no higher packing density than the one obtained for fcc and ideal hcp structures.
- **Thomas Hales** reported a computer-aided proof in 1998 (certain subsets of the problem were solved by the computer). The publication of the report delayed due to the complex reviewing process by the peers. Finally in 2005, the proof was published without a final decision by the reviewers on the correctness of the proof. Nevertheless, the reviewers stated to be 99% sure about the correctness.
- The Hales‘ group published results on a formal proof in 2017 (again computer-aided).

T. Hales: „A proof of the Kepler conjecture” Annals of Mathematics 162 (2005) 1065-1185
T. Hales, et al.: „A formal proof of the Kepler conjecture“ Forum of Mathematics 5 (2017) e2
http://www.sci-news.com/othersciences/mathematics/formal-proof-kepler-conjecture-04960.html

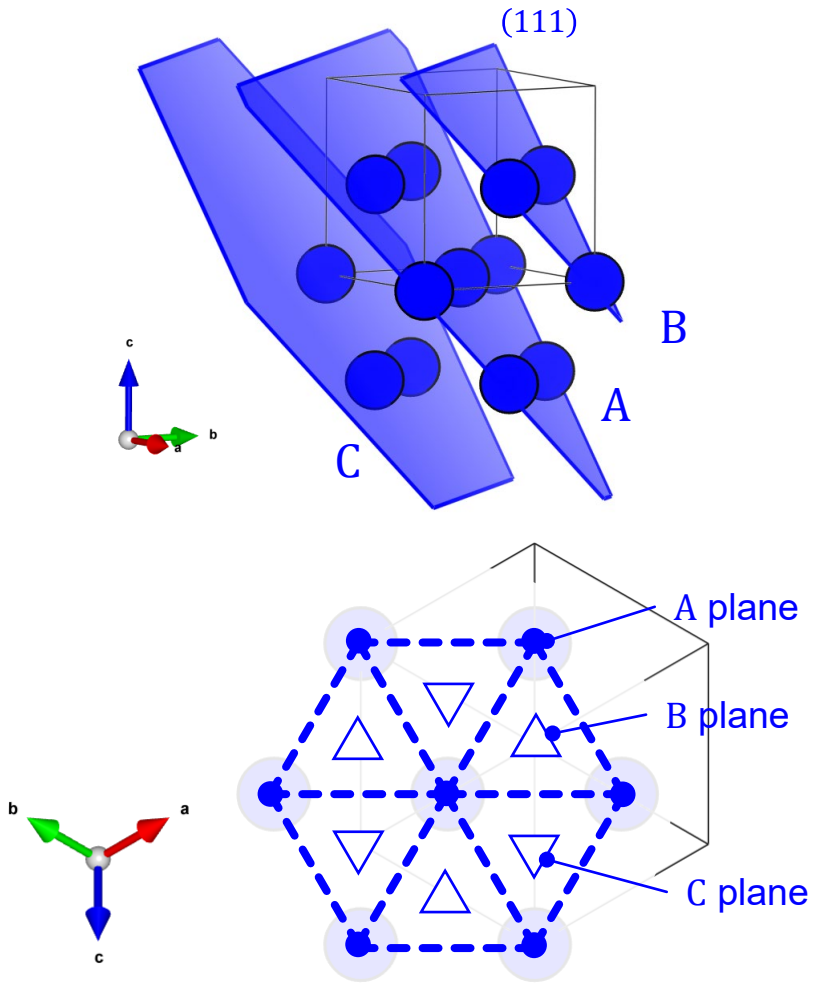
Stacking Sequences

Mg: ... ABABAB ...



Stacking Sequences

Cu: ... ABCABCABC ...



Stacking Faults

- It is easy to see, that there is an infinite number of possible stacking sequences apart from the two shown on the slides before; these are just the simplest versions of stacking.
- Later in the lecture, we will intensively discuss lattice defects and their relevance to plasticity. Particularly, we will discuss **stacking faults** which are **planar faults by changing stacking sequences**.
- **Extrinsic stacking faults** refer to **additional planes in stacking sequences**, whereas **intrinsic faults** refer to **missing planes in the sequence**.

Examples

Metal	Crystal System	Bravais Type	Prototype	Struktur-bericht	Space Group	Occ. Wyckoff Pos.	Lattice Param. at RT (in Å)	ICSD Collection Code
Cu	cub	fcc	Cu	A1	$Fm\bar{3}m$	4a	3.615	43493
Al							4.049	64700
Au							4.078	611623
Ni							3.524	64989
γ-Fe							–	–
α-Fe		bcc	W	A2	$Im\bar{3}m$	2a	2.866	53451
W							3.165	44323
β-Ti							–	–
Mg	hex	hex	Mg	A3	$P6_3/mcm$	2c	3.209 / 5.210 (c/a = 1.624)	76145
Zn							2.665 / 4.946 (c/a = 1.856)	653501
α-Ti							2.951 / 4.684 (c/a = 1.587)	43416

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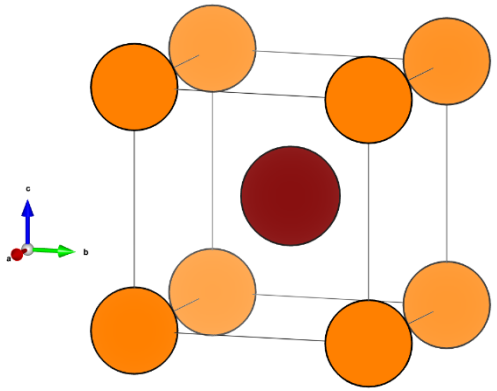
Note: hcp is not a Bravais type of lattice; it's a distinct description of a crystal structure.

Intermetallic Compounds

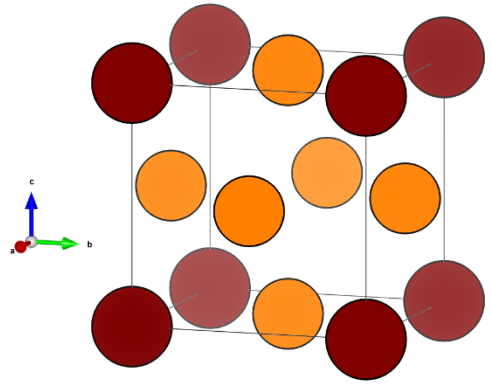
- Intermetallic compounds result from strong interaction of unlike atoms. In regular solution theory (see for example lecture “Phase Transformations in Materials”), this corresponds to $\varepsilon \ll 0$. This results in a high degree of order.
- Following structures are important for the lecture:

Prototype	Strukturbericht	Examples
CsCl	**B2**	NiAl, FeAl, etc.
Cu_3Au	**$L1_2$**	Ni_3Al
CuAu	**$L1_0$**	TiAl
Ni_3Sn	**$D0_{19}$**	**Ti_3Al**

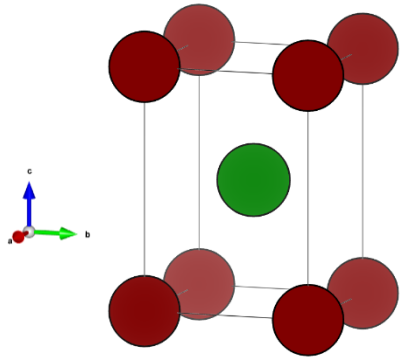
Intermetallic Compounds



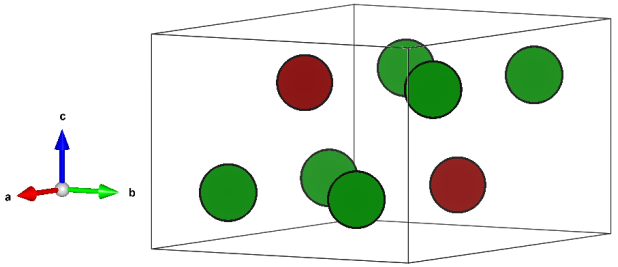
NiAl, B2



Ni_3Al, $L1_2$



TiAl, $L1_0$

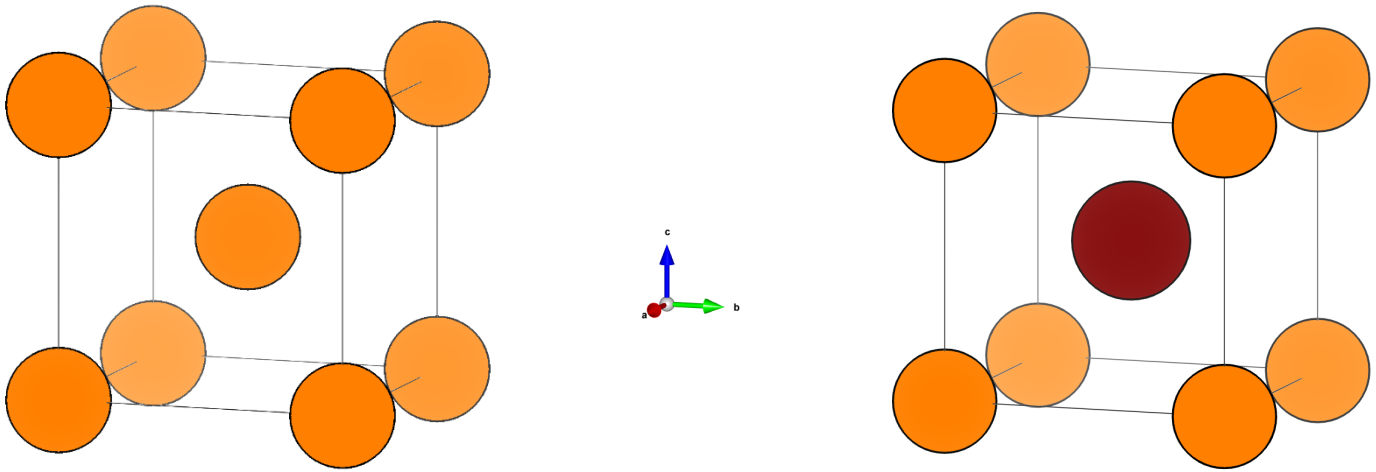


Ti_3Al, $D0_{19}$

Intermetallic Compounds

- Due to the order principles, significant similarities can be found between intermetallic compounds and disordered solid solutions. We will utilize this analogy in order to describe the mechanical behavior:

for example: Fe und FeAl

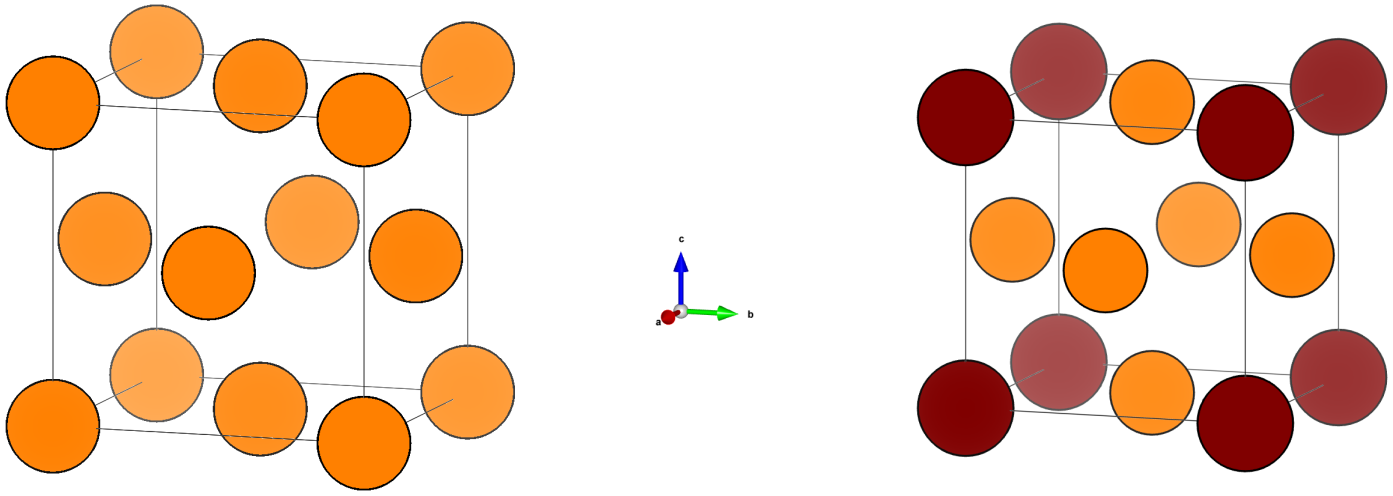


A2 **B2**

Intermetallic Compounds

- Due to the order principles, significant similarities can be found between intermetallic compounds and disordered solid solutions. We will utilize this analogy in order to describe the mechanical behavior:

for example Ni und Ni_3Al

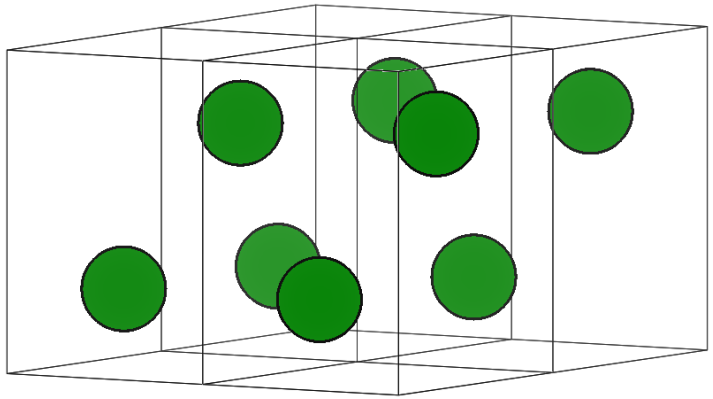


A1 **$L1_2$**

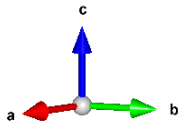
Intermetallic Compounds

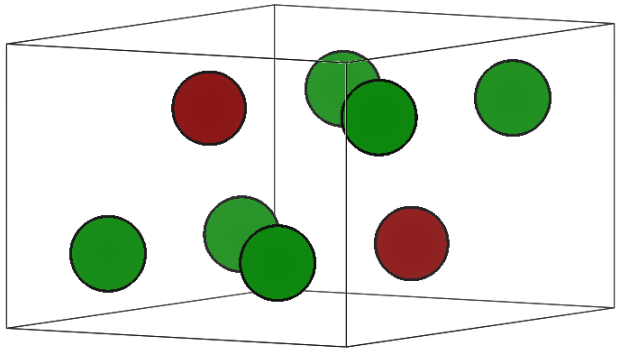
- Due to the order principles, significant similarities can be found between intermetallic compounds and disordered solid solutions. We will utilize this analogy in order to describe the mechanical behavior:

for example Ti und Ti_3Al



A3





$D0_{19}$

Note that the hcp Ti unit cell was rotated for better comparison.

Examples

Inter.	Crystal System	Bravais Type	Prototype	Struktur-bericht	Space Group	Occ. Wyckoff Pos.	Lattice Param. at RT (in Å)	ICSD Collection Code
NiAl	cub	sc	CsCl	B2	$Pm\bar{3}m$	1a, 1b	2.885	191110
FeAl							2.910	165164
Ni_3Al	cub	sc	Cu_3Au	$L1_2$	$Pm\bar{3}m$	1a, 3c	3.572	58038
TiAl	tetr	st	CuAu	$L1_0$	$P4/mmm$	1a, 1d	2.829 / 4.071	107891
Ti_3Al	hex	hex	Ni_3Sn	$D0_{19}$	$P6_3/mmc$	2c, 6h	5.764 / 4.664	99779

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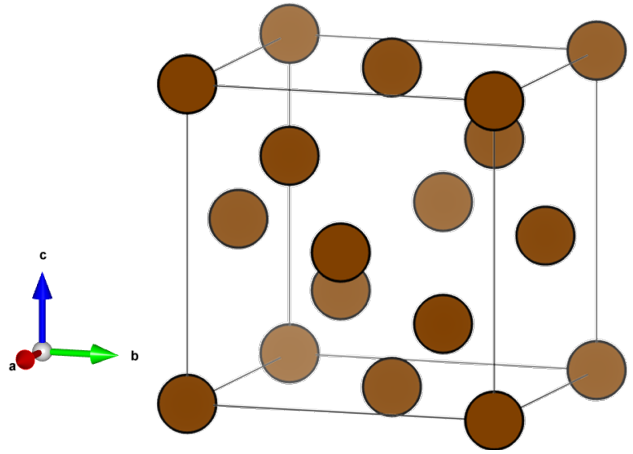
Other Materials

- In covalent or ionic materials, the structure principles are different from metallic materials since the binding is directional or balance of charge is necessary.
- Following structures are important to the lecture:

Prototype	Strukturbericht	Examples
Diamond	**A4**	diamond, Si, Ge, etc.
NaCl	**B1**	NaCl

Other Materials



diamond

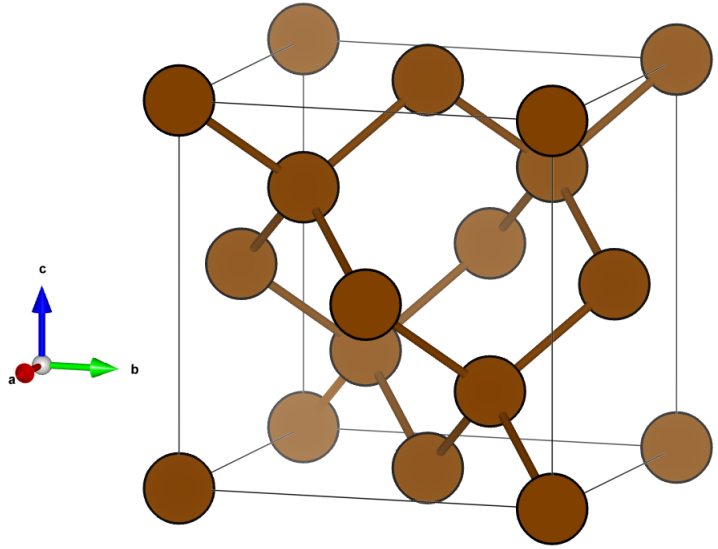
coordination: 4

no. of atoms in the unit cell: $4 \cdot 1 + 8 \cdot \frac{1}{8} + 6 \cdot \frac{1}{2} = 8$

atomic packing factor: $34\ \%$

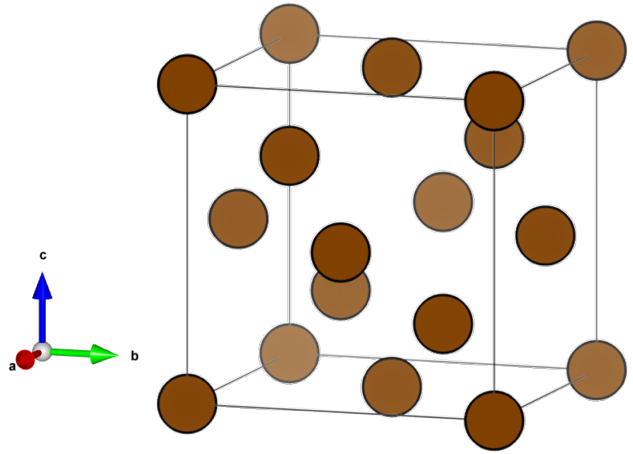
densely packed directions: $\langle 111 \rangle$

densely packed planes: $\{110\}$

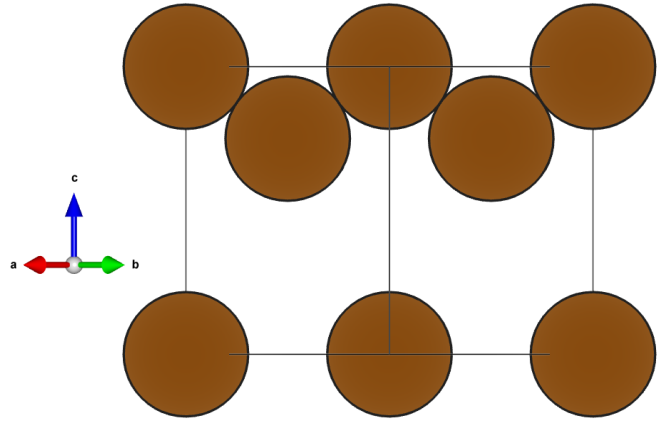


- The coordination determined by the covalent binding is a tetrahedron.
- There are two sub-lattices of Cu structure type which are displaced by ¼ of the body diagonal of the unit cell.

Other Materials



diamond
coordination: 4
no. of atoms in the unit cell: 8
atomic packing factor: 34 %
densely packed directions: ⟨111⟩
densely packed planes: {110}

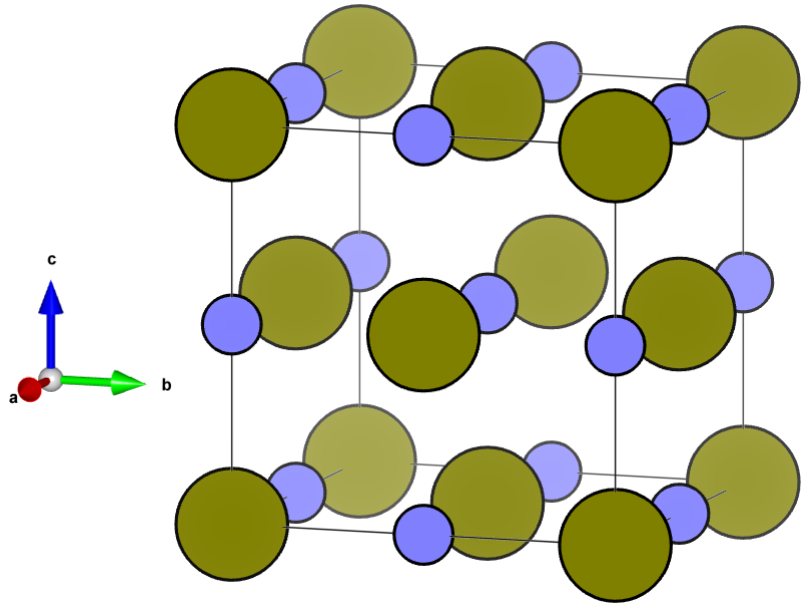


$$PF = \frac{N_\mathrm{a} \cdot V_\mathrm{a}}{V_\mathrm{uc}} = \frac{8 \cdot \frac{4}{3}\pi R^3}{a^3}$$

$$2R = \frac{1}{4}\sqrt{3}a$$

$$PD = \frac{\sqrt{3}}{16}\pi$$

Other Materials



NaCl, B1

Examples

Phase	Crystal System	Bravais Type	Prototype	Struktur-bericht	Space Group	Occ. Wyckoff Pos.	Lattice Param. at RT (in Å)	ICSD Collection Code
Si	cub	fcc	**Diamond**	**A4**	$Fd\bar{3}m$	8a	5.431	51688
NaCl	cub	fcc	**NaCl**	**B1**	$Fm\bar{3}m$	4a, 4b	5.642	181148

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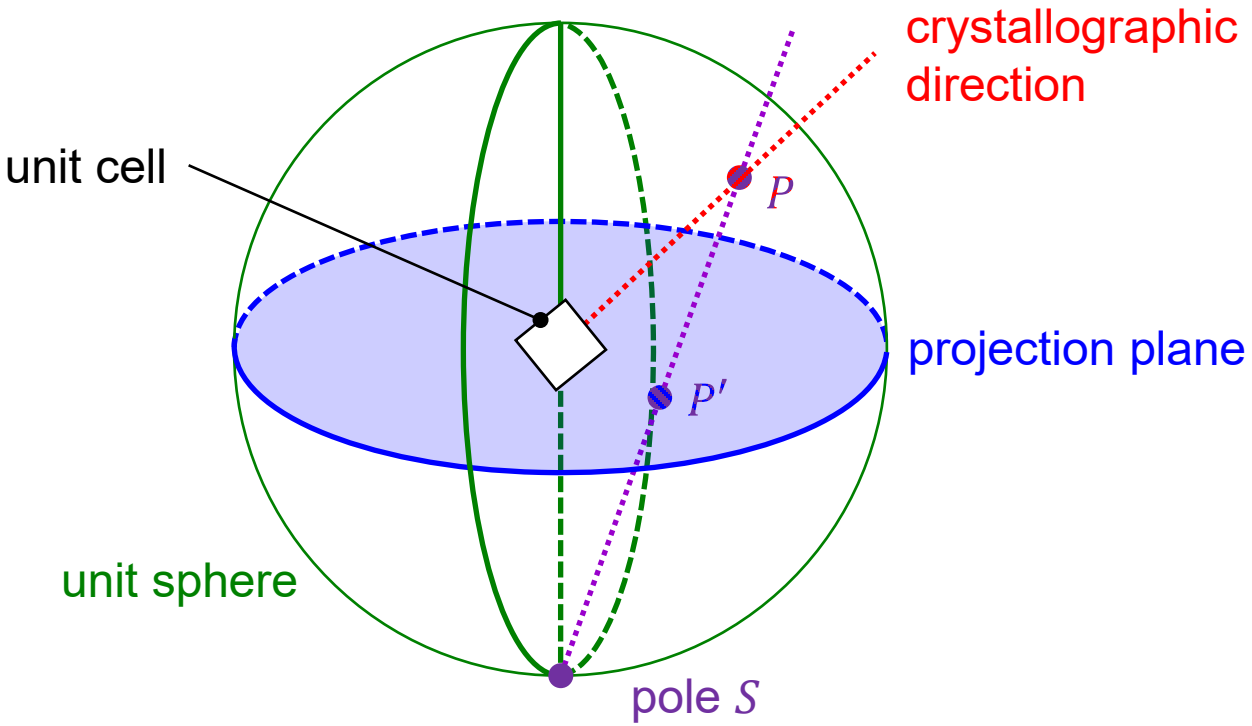
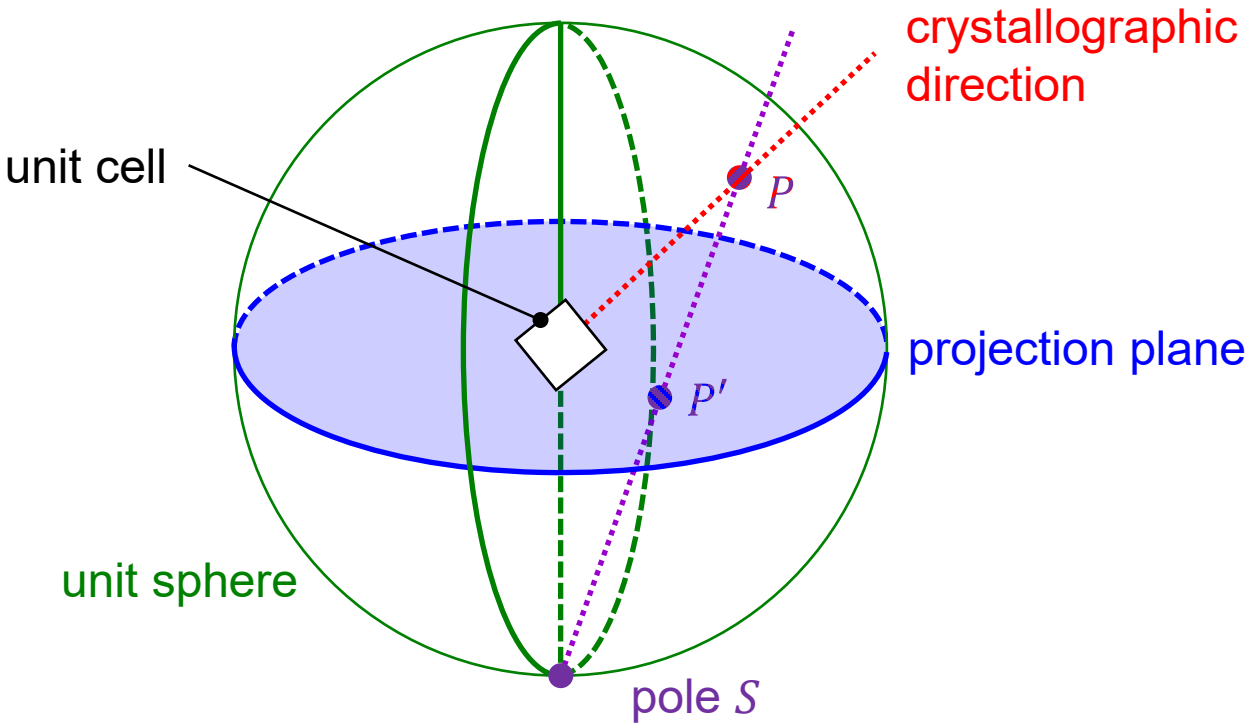
Stereographic Projection

- In order to efficiently visualize many directions and plane normals in 2D, proper projections are necessary. There are many different projections with various drawbacks and advantages available. The **stereographic projection** is frequently applied in our discipline:



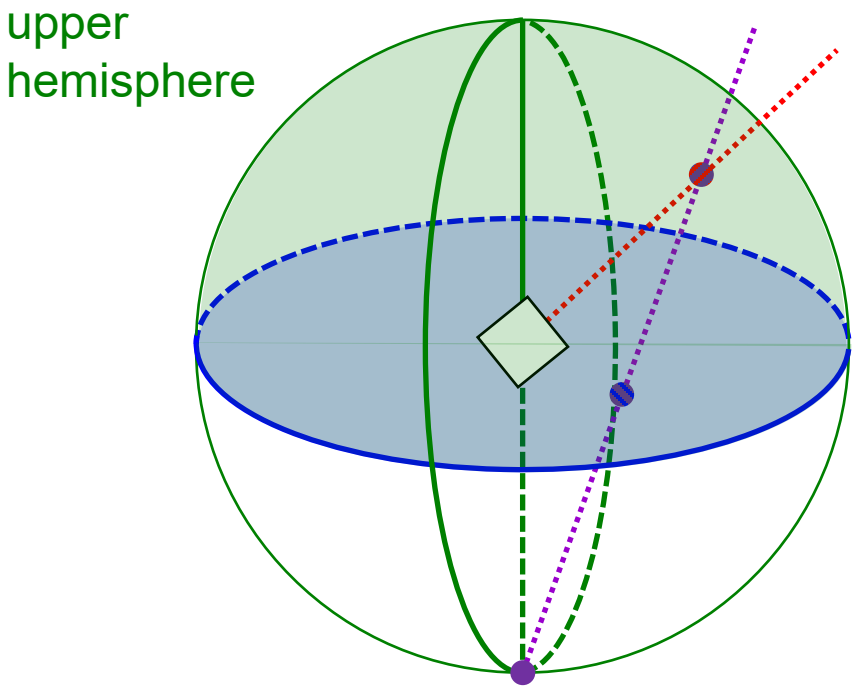
Stereographic Projection

- A crystallographic direction or plane normal has a certain intersection point P with the unit sphere. The mapping P' of the direction or plane normal is given by the intersection of a plane (usually the equatorial plane) and the line connecting one pole S (typically “south”) with P.



Stereographic Projection

- In most cases, only the upper hemisphere is mapped. Often, the exact mapping rule is ignored and lower hemisphere is projected towards the opposite pole (equ. to fold over to the upper hemisphere.). Strictly, the lower hemisphere is outside the unit circle!

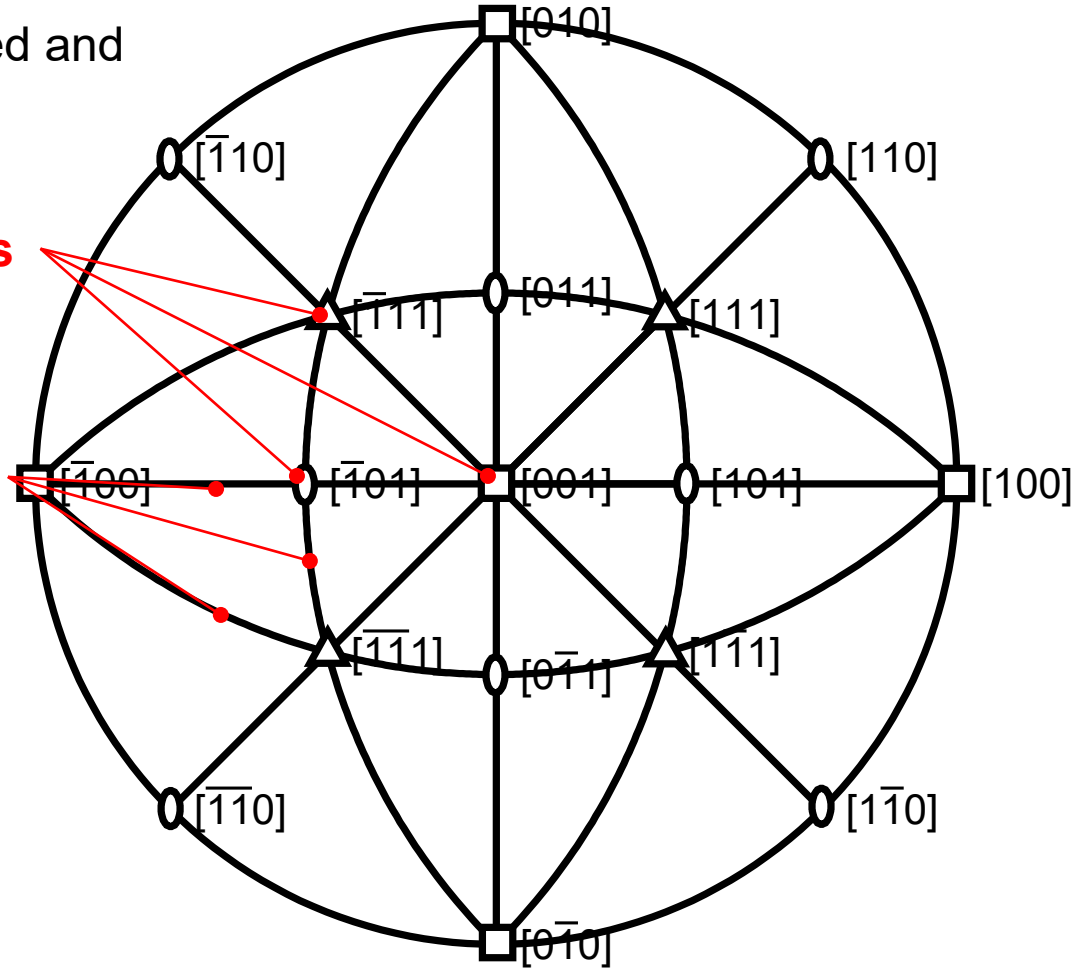


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

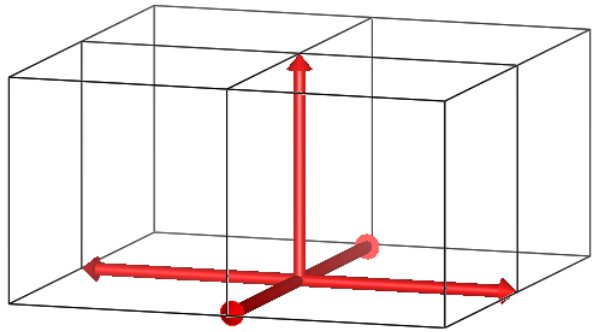
projection of specific directions

projection of all directions covered by a rotation from one distinct direction to another

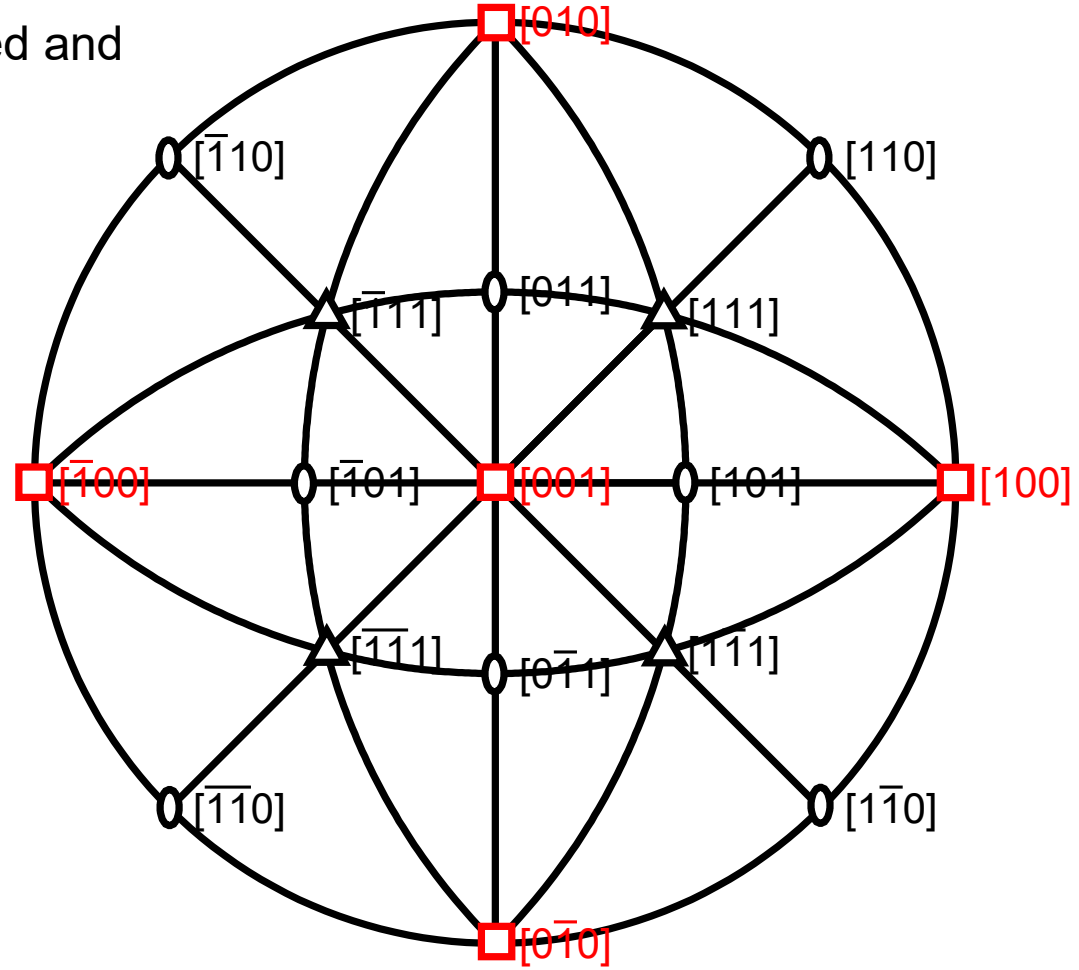


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

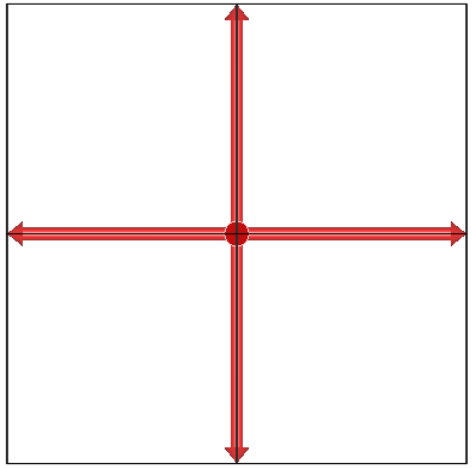


The ⟨100⟩ are 4-fold axes (□)

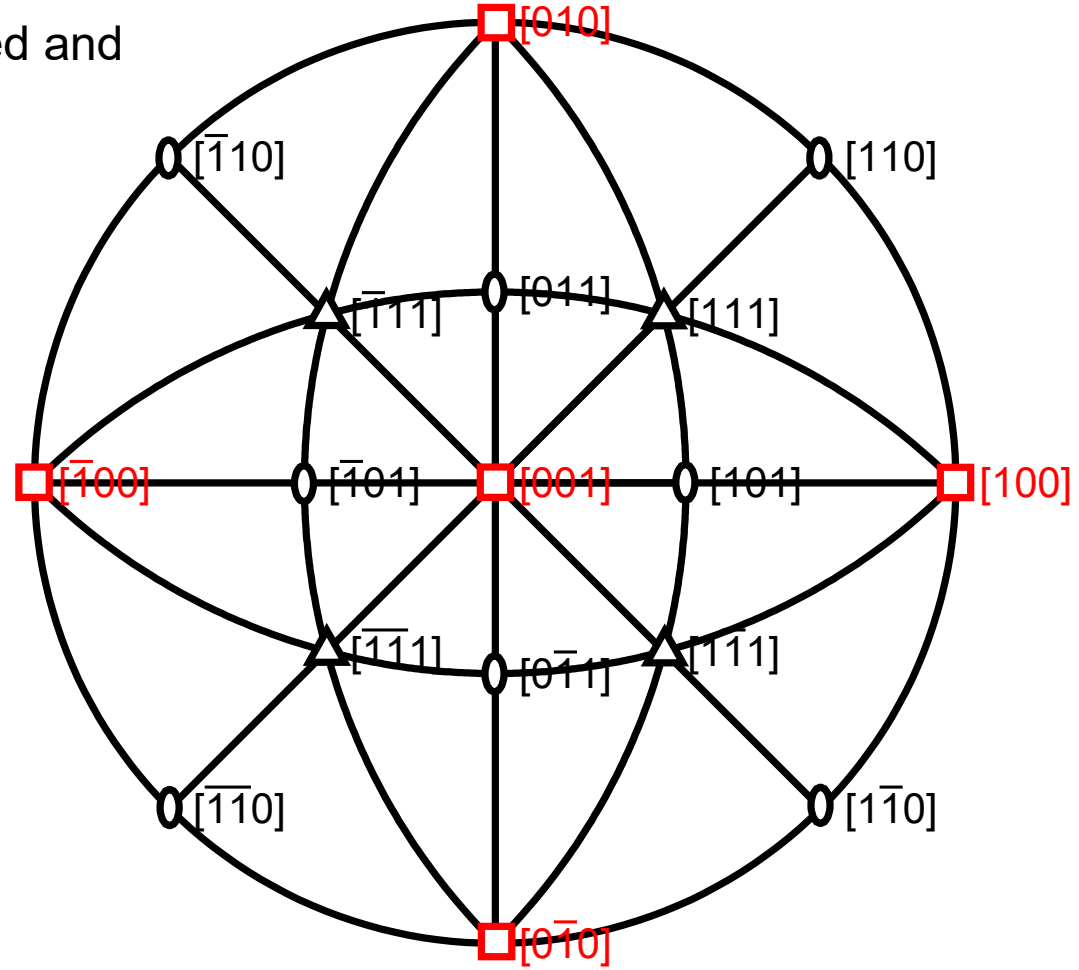


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

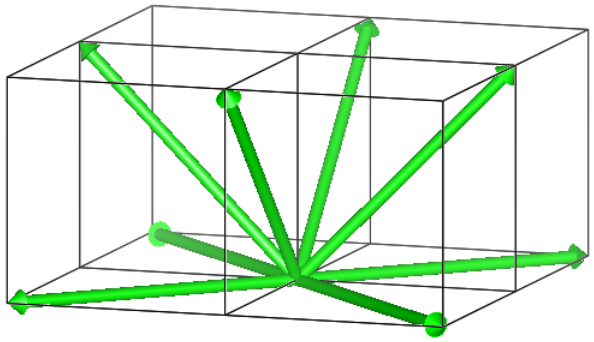


Top view, looking from $[001]$.

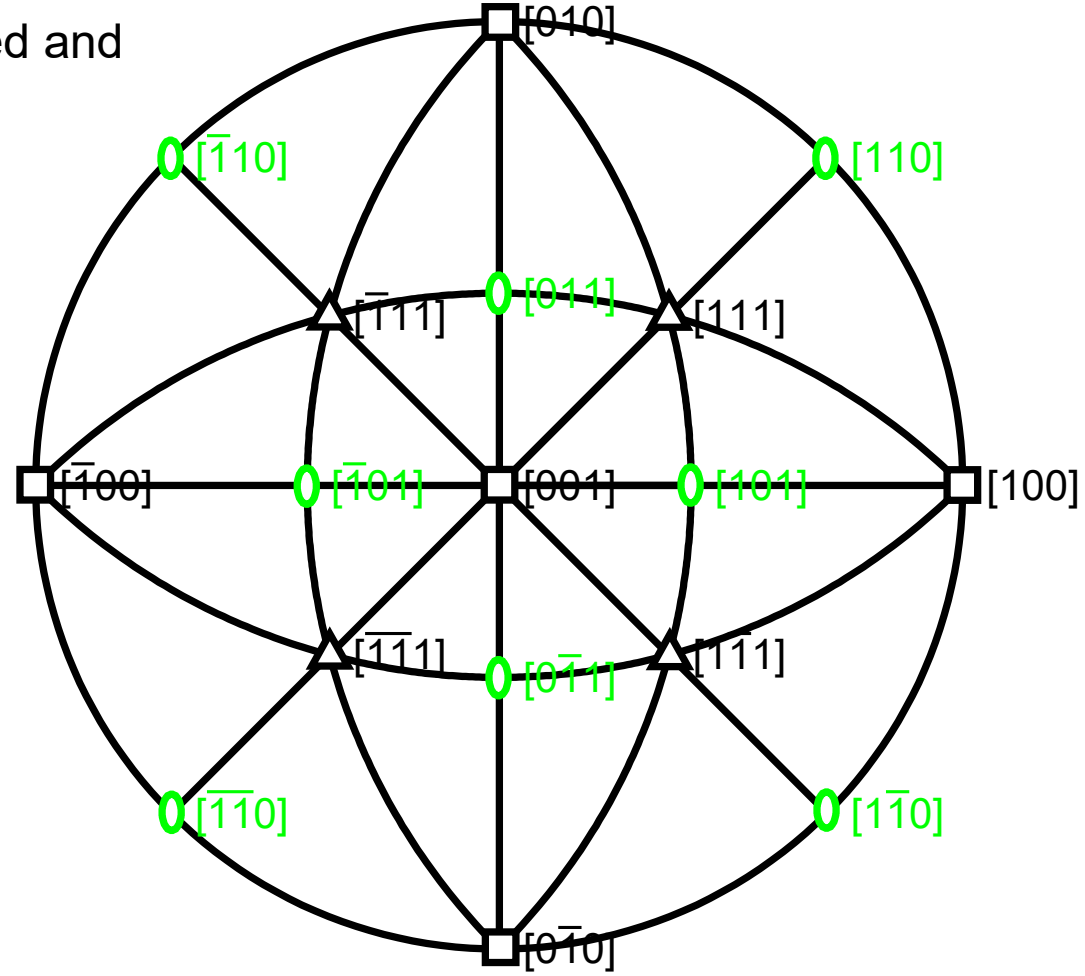


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

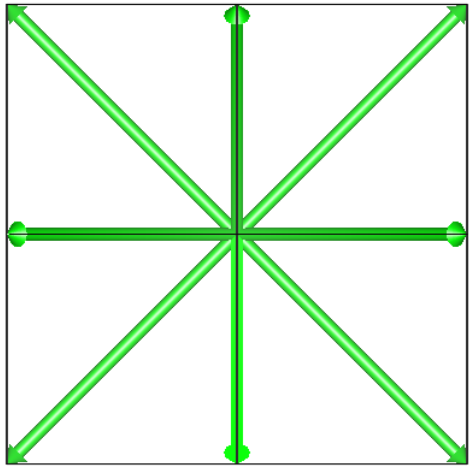


The ⟨110⟩ are 2-fold axes (0)

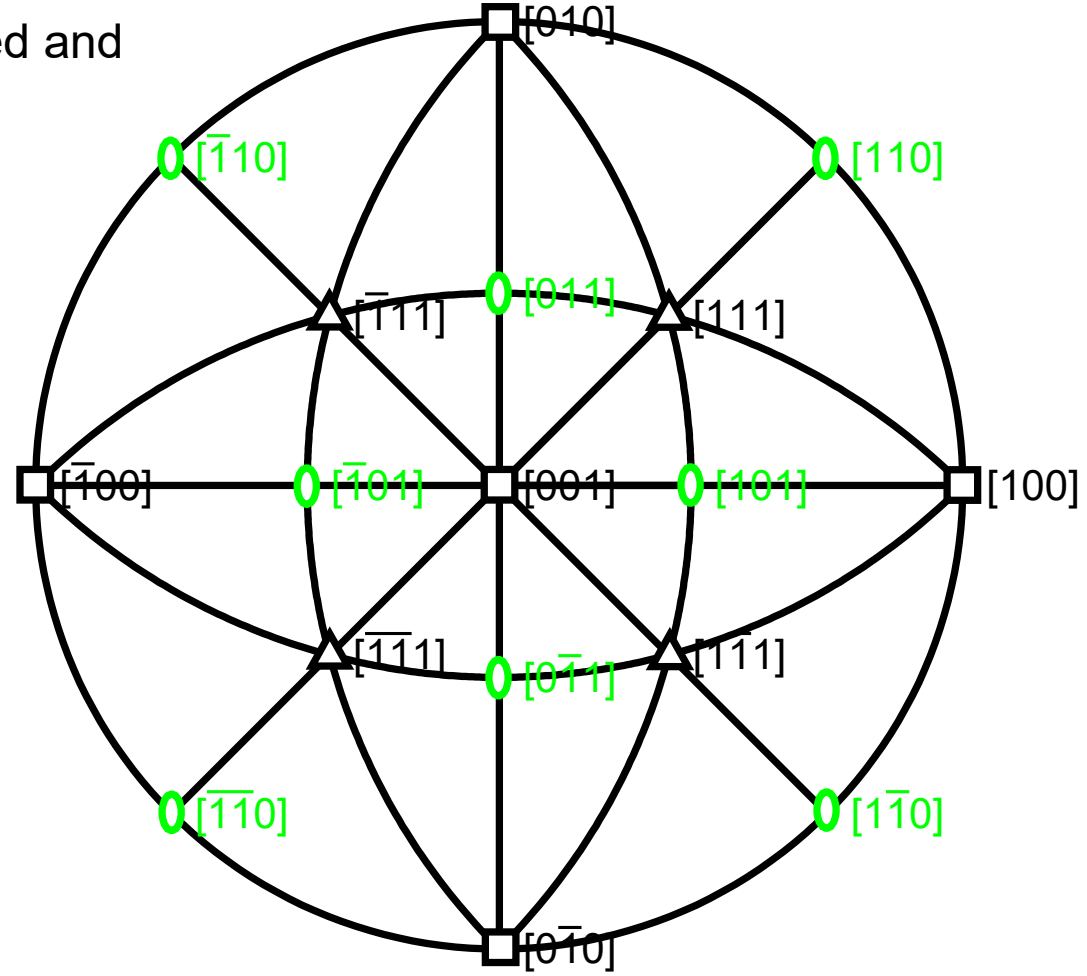


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

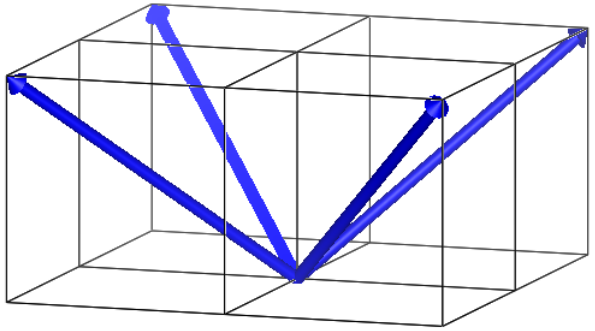


Top view, looking from $[001]$.

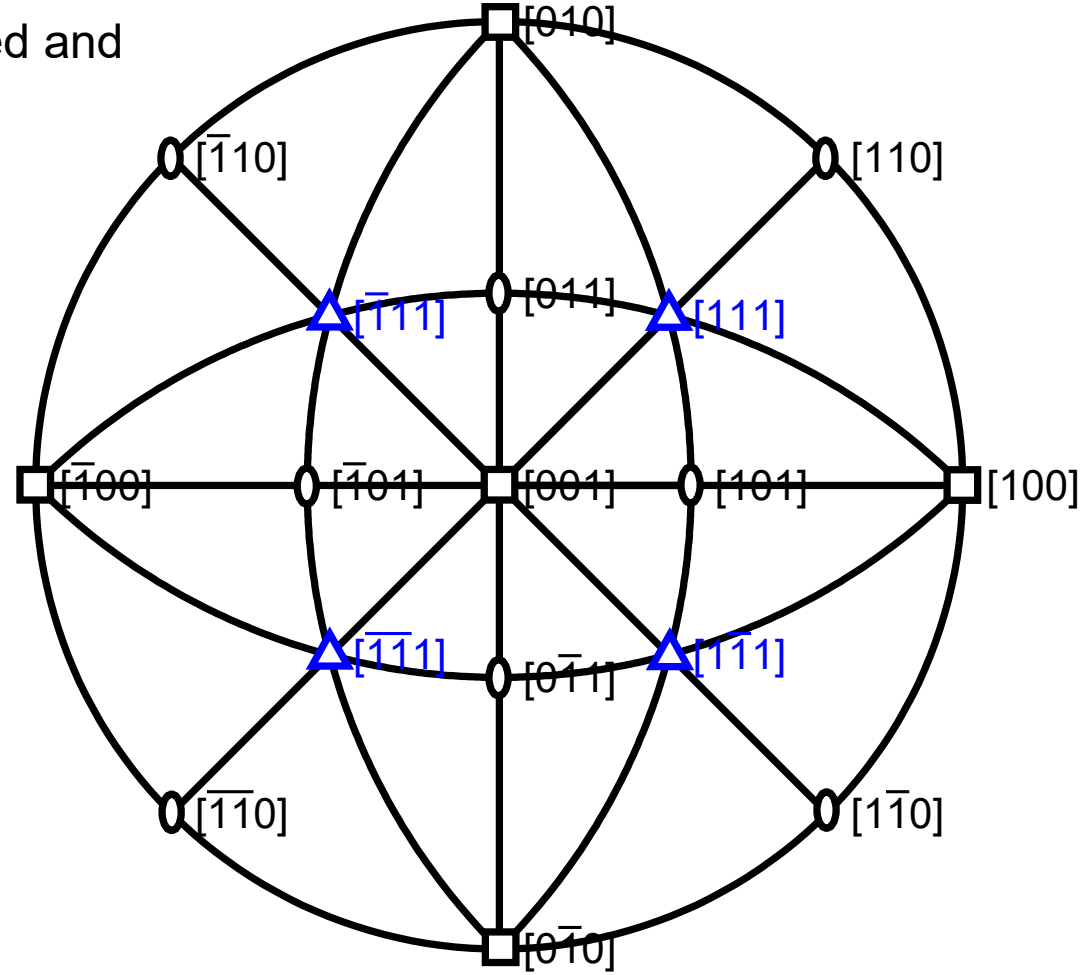


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

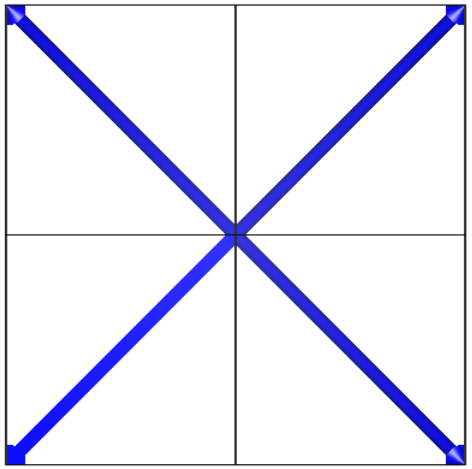


The $\langle 111 \rangle$ are 3-fold axes (Δ) and characteristic of cubic systems!

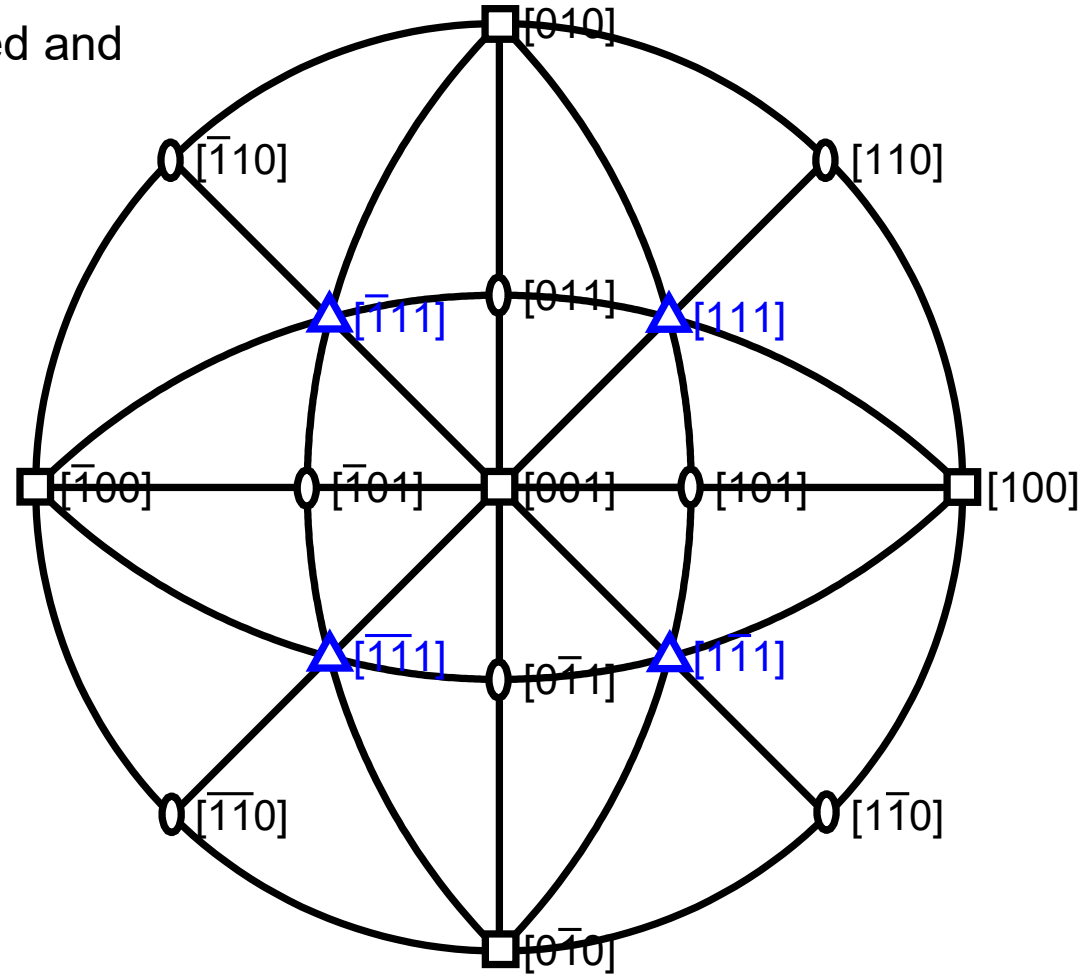


Stereographic Projection

- Example: all cubic crystals (specifically placed and oriented within the unit sphere)

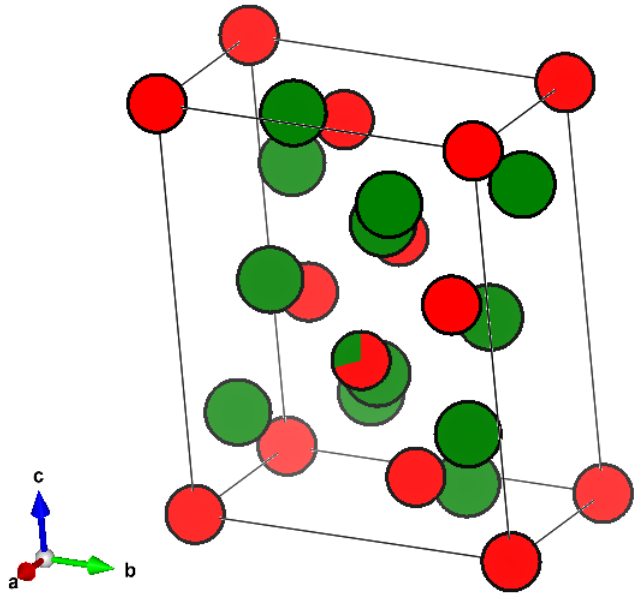


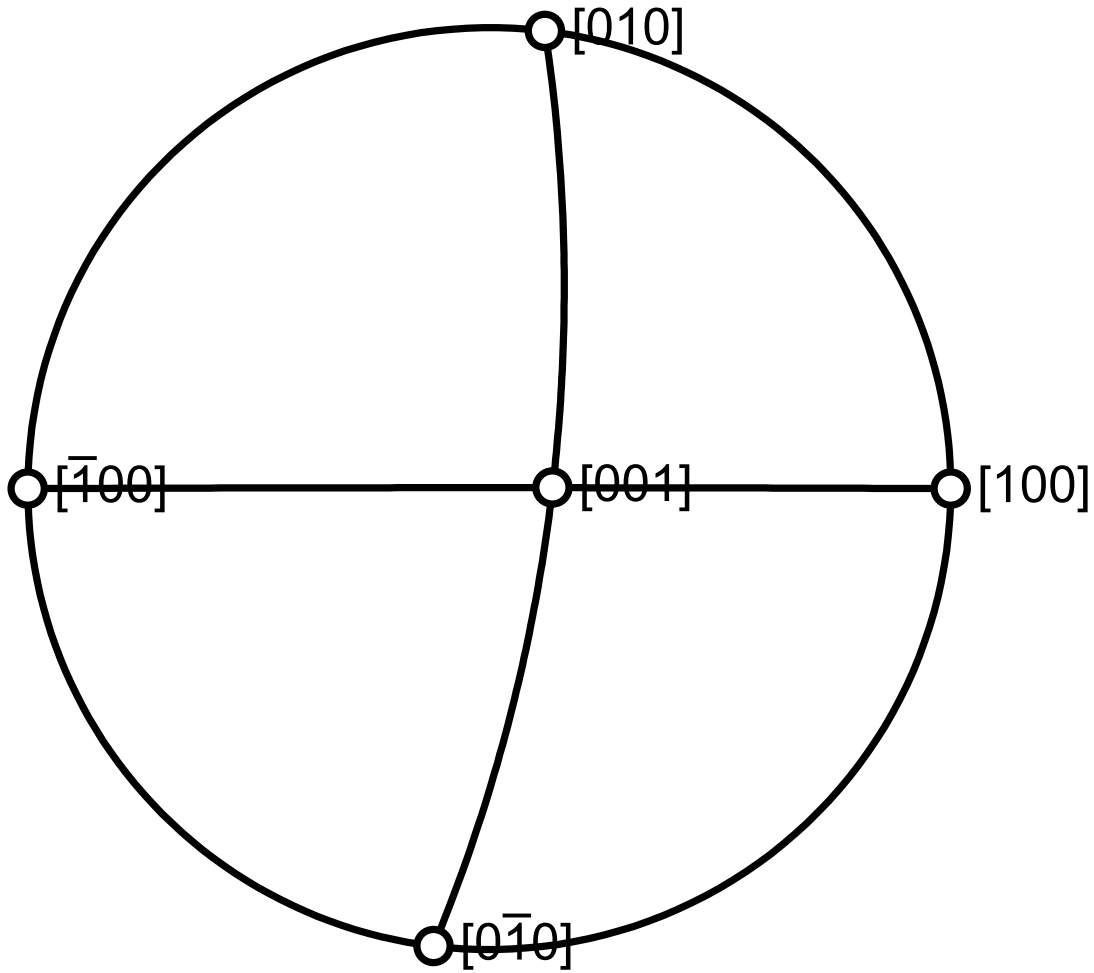
Top view, looking from $[001]$.



Stereographic Projection

- Example:
  $FeAl_2$, triclinic
  $a = 4.875$ Å, $b = 6.455$ Å, $c = 8.736$ Å
  $\alpha = 87.93°$, $\beta = 74.40°$, $\gamma = 83.06°$





Stereographic Projection

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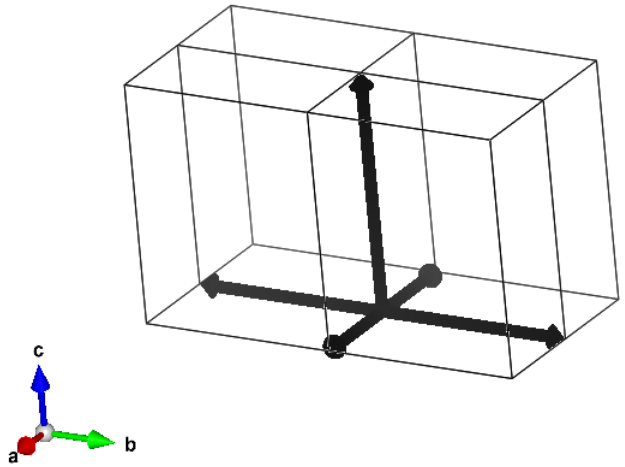
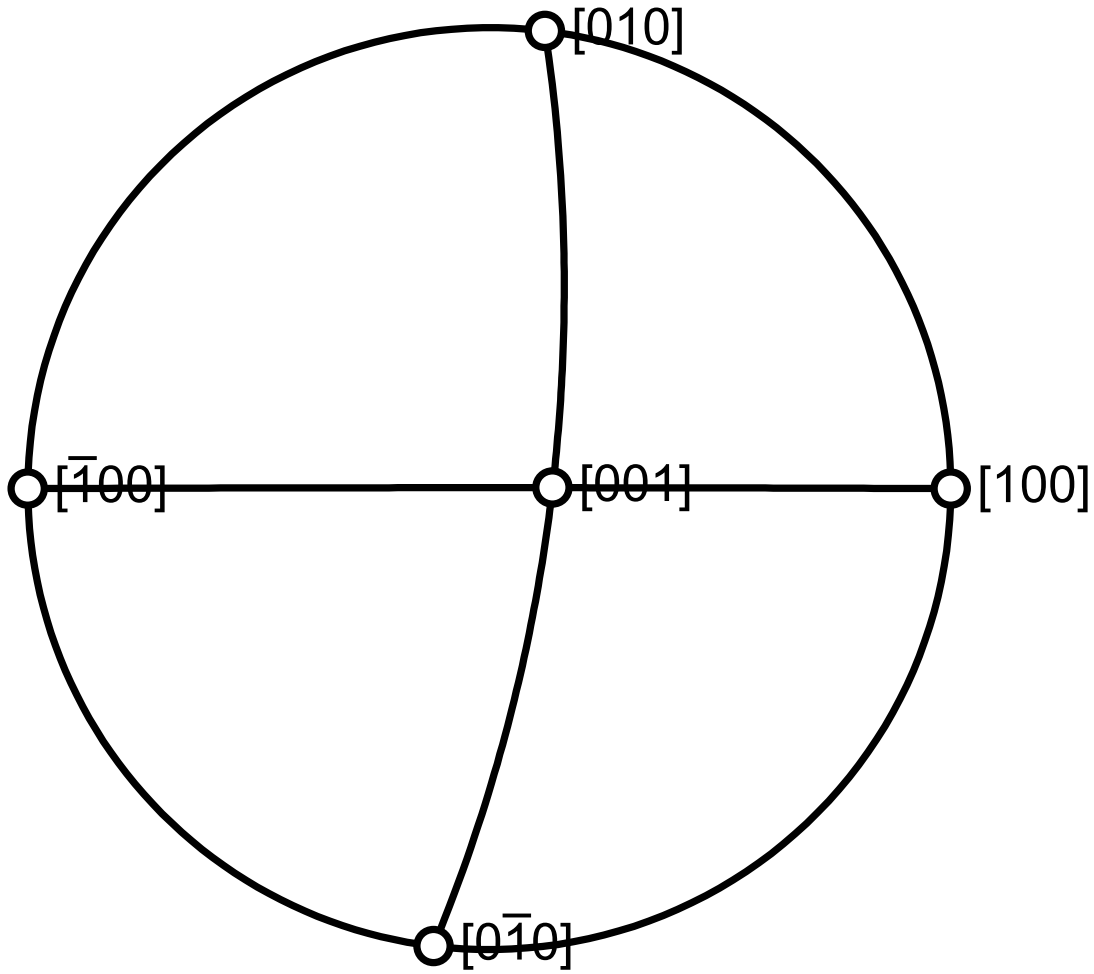


only: 1 (no symmetry) or $\bar{1}$ (inversion center)



Stereographic Projection

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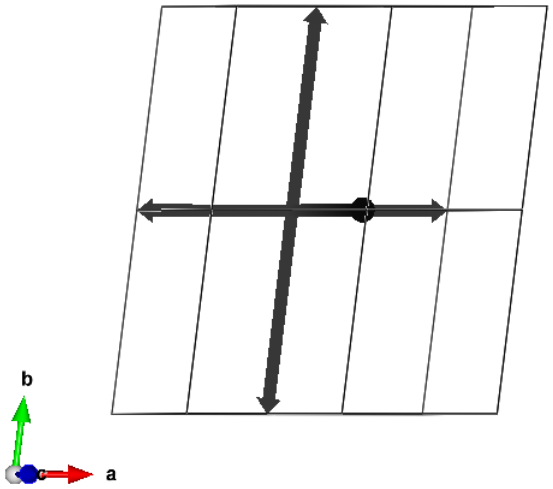
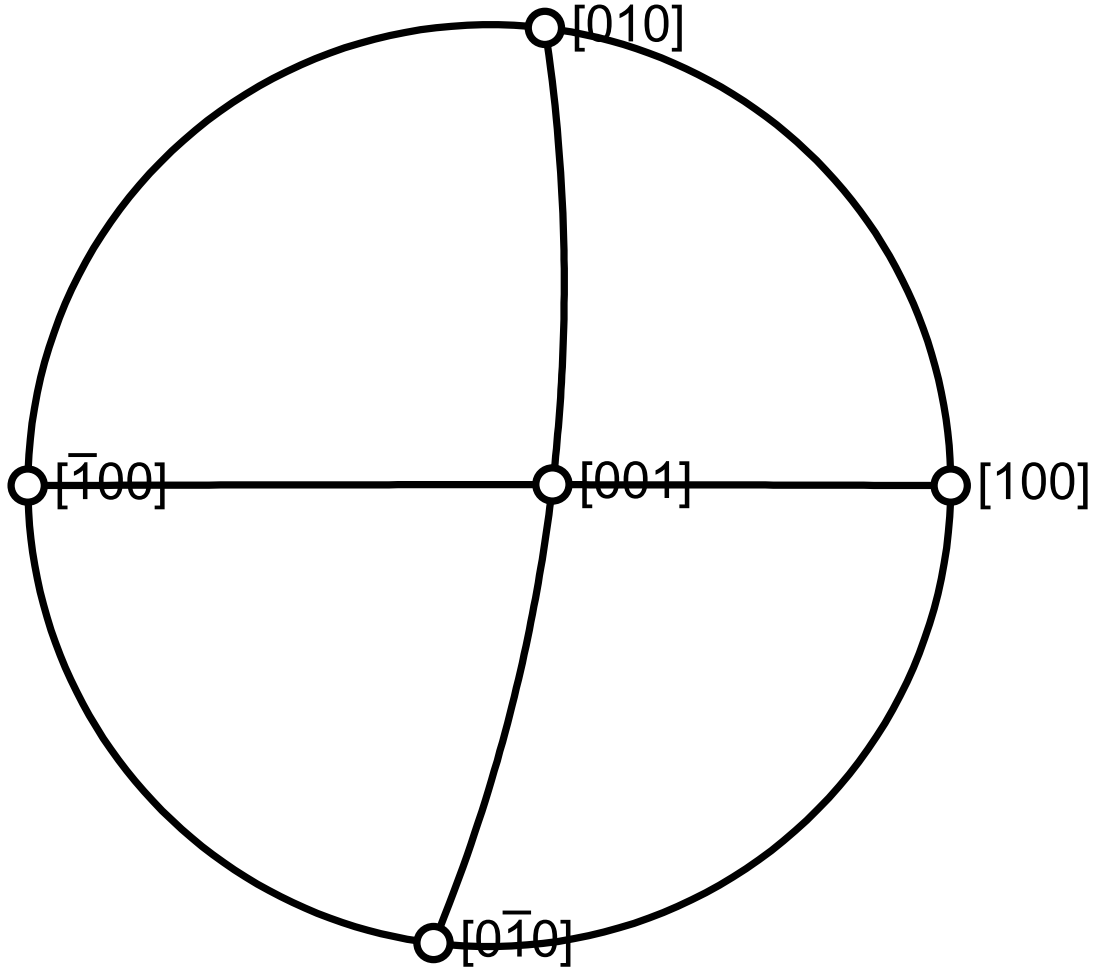


view onto (001)

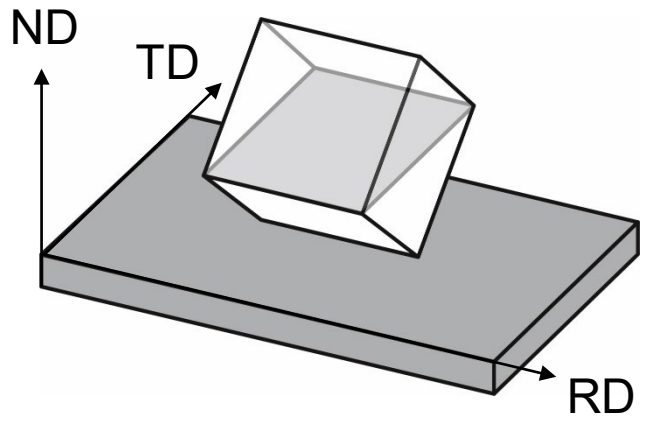


Texture Components

- **An orientation is a transform from one coordinate system into another.** In materials science, it is in most cases a **transform from the crystal system into the sample system or vice versa.**
- The unit sphere of the stereographic projection can be aligned with respect to the sample system, since it is often Cartesian. For example the sample system for rolling is rolling direction (RD), normal direction (ND) and transversal direction (TD).
- When the unit sphere is aligned with the sample system and visualizes the **mapping of the crystal system with respect to the sample system**, we call this projection **pole figure**.
- An **inverse pole figure** displays the **sample system with respect to the** aligned **crystal system**.

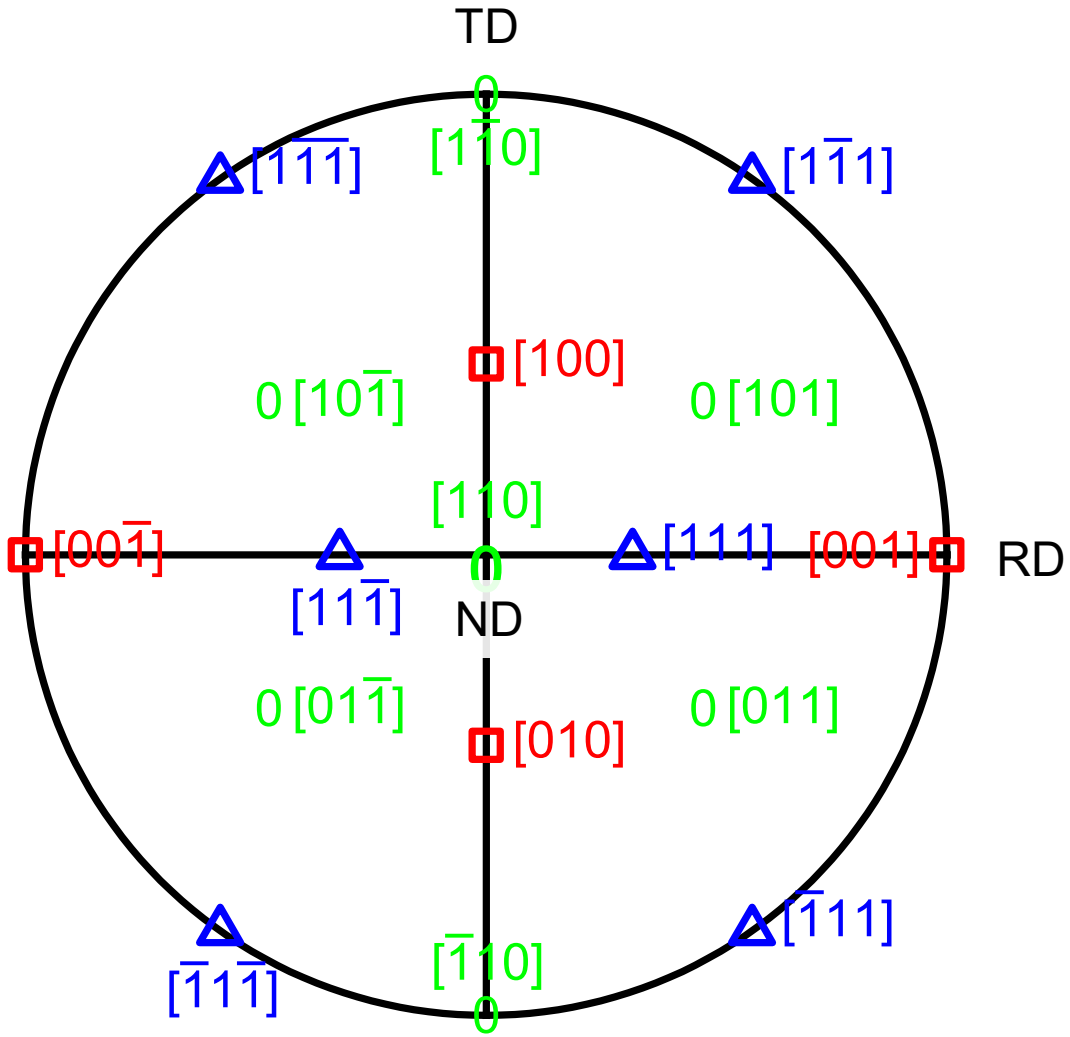
Visualization of Orientations

- Example:
  Goss, for example in
  bcc, soft-magnetic Fe-Si
  transformer sheets



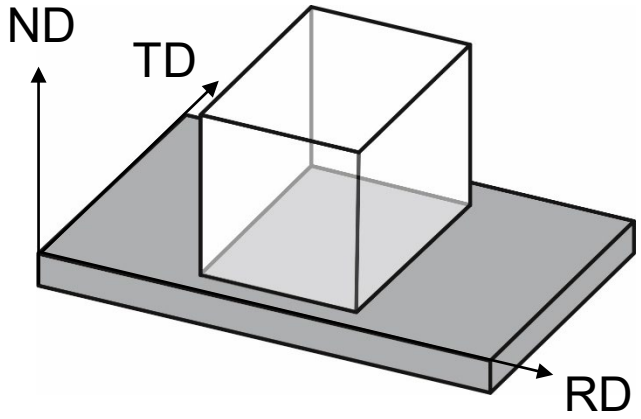
$\{110\}\langle 001\rangle$

(first plane within the rolling plane, second direction parallel to rolling direction)

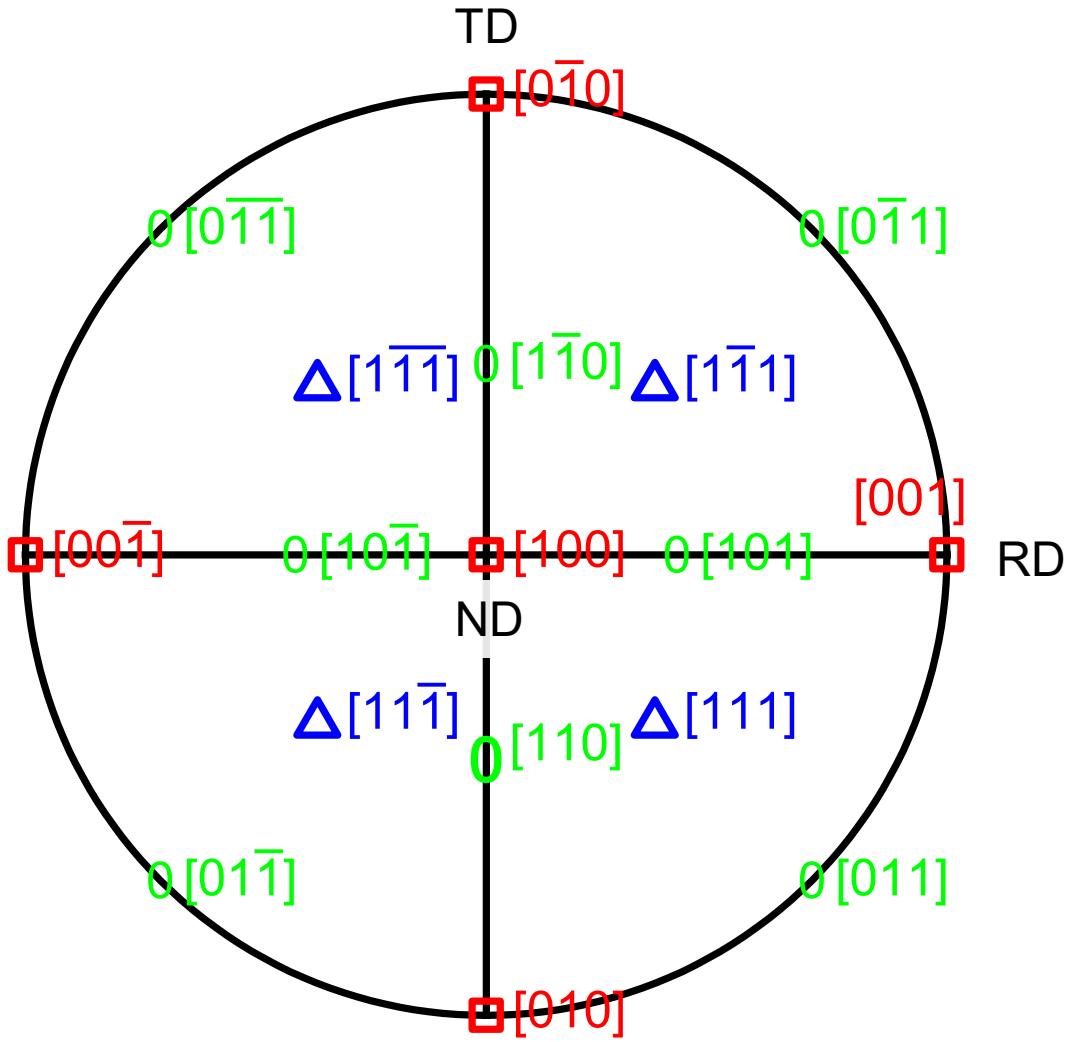


Visualization of Orientations

- Example:
  Cube, for example in rolling assisted biaxially textured substrates for superconducting thin films (RABiTs)



$\{100\}\langle 001\rangle$
(first plane within the rolling plane, second direction parallel to rolling direction)



Summary

- **Crystalline materials** usually exhibit **translational symmetry**. The **description of crystals** is performed using a **point lattice and** a **basis of atoms** or molecules.
- **crystallographic directions** and **lattice planes** can be described with respect to the **crystal system** (right-handed axial reference).
- Over the curse of the lecture, we will mainly use **structure types** and **Strukturbericht** designation.

Common Short Notations: Pearson Symbol

- **Crystal system + centering + number of atoms in the conventional cell**
- With
  a = triclinic, m = monoclinic, o = orthorhombic, t = tetragonal, h = hexagonal/trigonal, c = cubic
  and
  P = primitive, S = base centered (A, B und C), R = rhombohedral, F = face centered, I = body centered

Pearson Symbol	Prototypes
cF4	Cu
cI2	W
hP6	Mg
cF8	Diamond
cI58	α-Mn
cF8	NaCl
cP2	CsCl
hP12	$MgZn_2$ Laves phase
cF24	Cu_2Mg Laves phase
hP24	$MgNi_2$ Laves phase

…

Symmetry

- A dominating factor of modern crystallography is the application and description of symmetries
- Symmetries determine fundamental materials properties
- Symmetry elements (points, lines, planes) are used about which symmetry operations take place

Symmetry Element	Symmetry Operation	Symbol	Description
Identity		1	
Inversion center	Inversion	$\bar{1}$	Point mirroring
Axis of Rotation	Rotation	$2, 3, 4, (5), 6, (10)$	Rotation by $360°/n$
Mirror plane	Mirroring	m	Mirroring at a mirror plane
Rotoinversion Axis	Rotoinversion	$\bar{2}, \bar{3}, \bar{4}, \bar{6}$	Coupled rotation and inversion
Rotating mirror axis	Rotating mirroring	$2/\mathrm{m}, 3/\mathrm{m}, 4/\mathrm{m}, 6/\mathrm{m}$	Rotation perpendicular to the mirror plane
Glide plane	Glide mirroring	$\mathrm{a}, \mathrm{b}, \mathrm{c}$	Mirrroring with translation along half a basis vector
Glide plane	Glide mirroring	n	Mirroring with translation along half a surface diagonal
Glide plane	Glide mirroring	e	Two glide mirrors with the same glide mirror plane and translation along two (different) half lattice vectors
Screw axis		$2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1, 6_5, 6_2, 6_4, 6_3$	n_m results in n-fold rotation with translation by m/n parts of a lattice vector

Point Groups

- **Point groups (sometimes referred to as crystal classes)** are **groups of symmetry operations** that are applied to **objects of finite geometry**.
- In the case of crystallography, point groups describe the shape of crystals.
- **32 crystallographic point groups exist**.

Crystal System	Point Groups (H-M notation)						
cubic	23	$m\bar{3}$		432	$\bar{4}3m$	$m\bar{3}m$	
hexagonal	6	$\bar{6}$	6/m	622	6mm	$\bar{6}m2$	6/mmm
Trigonal	3	$\bar{3}$		32	3m	$\bar{3}m$	
tetragonal	4	$\bar{4}$	4/m	422	4mm	$\bar{4}2m$	4/mmm
orthorhombic				222		mm2	mmm
monoclinic	2		2/m		m		
triclinic	1	$\bar{1}$					

Space Groups

- **Space groups** are **groups of symmetry operations** that are applied to **infinite lattices/patterns**.
- **230 crystallographic space groups exist**.

Number	Crystal System	Point Group	Examples
1	triclinic (2)	1	P1
2		$\bar{1}$	P$\bar{1}$
3–5	monoclinic (13)	2	C2
6–9		m	Cc
10–15		2/m	P21/m
16–24	orthorhombic (59)	222	P222
25–46		mm2	Pmm2
47–74		mmm	Pmmm
75–80	tetragonal (68)	4	I41
81–82		$\bar{4}$	P$\bar{4}$
83–88		4/m	P4/m
89–98		422	I422
99–110		4mm	I4mm
111–122		$\bar{4}$2m	I$\bar{4}$m2
123–142		4/mmm	P4/mmm
143–146	trigonal (25)	3	R3
147–148		$\bar{3}$	P$\bar{3}$
149–155		32	P321
156–161		3m	R3c
162–167		$\bar{3}$m	R$\bar{3}$c
168–173	hexagonal (27)	6	P65
174		$\bar{6}$	P$\bar{6}$
175–176		6/m	P6/m
177–182		622	P622
183–186		6mm	P6mm
187–190		$\bar{6}$m2	P$\bar{6}$m2
191–194		6/mmm	P63/mmc
195–199	cubic (36)	23	I23
200–206		m$\bar{3}$	Im$\bar{3}$
207–214		432	P432
215–220		$\bar{4}$3m	F$\bar{4}$3m
221–230		m$\bar{3}$m	Pm$\bar{3}$m, Fm$\bar{3}$m, Im$\bar{3}$m

Space Groups

- When working with crystal structures, the use of space groups is important.
- Most relevant notations are:
  - Number according to the International Tables of Crystallography
  - Hermann-Mauguin notation

1st symbol: Bravais type of lattice
2nd … 4th symbol: symmetry elements along certain viewing directions

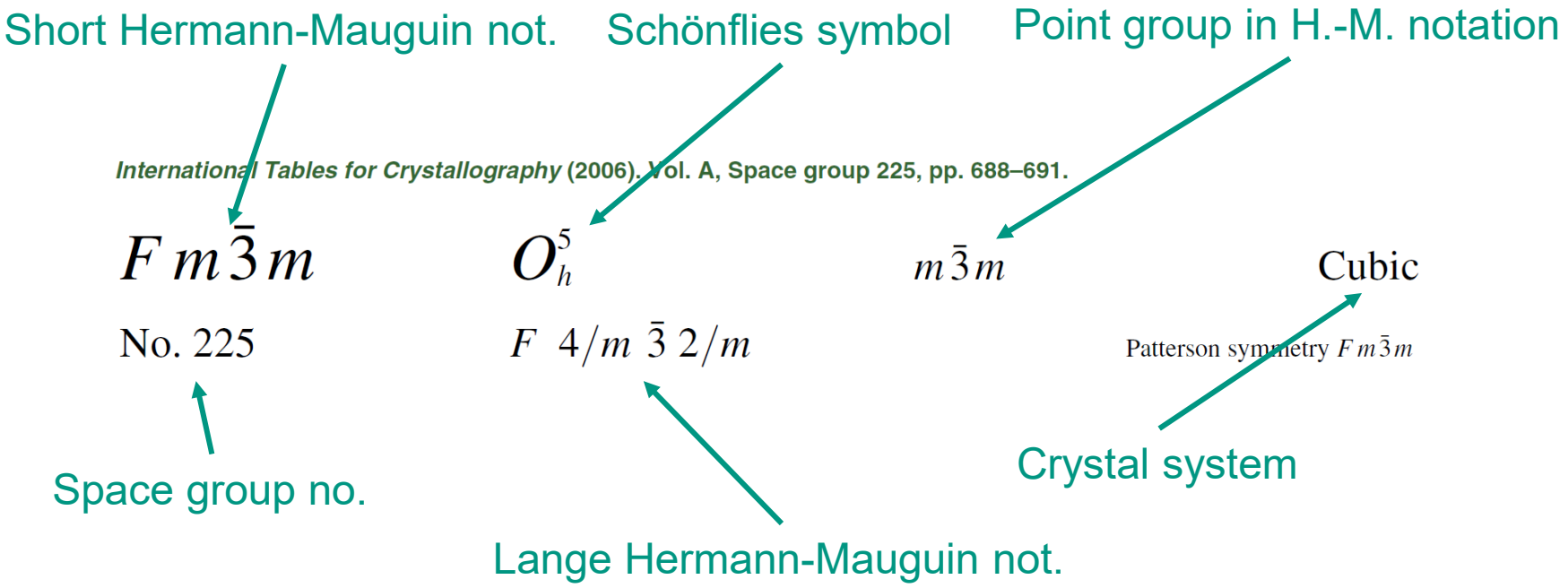
Crystal System	1st viewing direction	2nd viewing direction	3rd viewing direction	Characteristic
triclinic	-			1 or $\bar{1}$
monoclinic	[010] or [001]	-		2 or m on the 1st VD
orthorhombic	[100]	[010]	[001]	
tetragonal	[001]	[100] and [010]	[1-10] and [110]	4 on the 1st VD
trigonal	[111]	$[1\bar{1}0]$ or $[01\bar{1}]$ or $[\bar{1}01]$	-	3 on the 1st VD
hexagonal	[001]	[100] or [010] or $[\bar{1}\bar{1}0]$	$[1\bar{1}0]$ or $[\bar{1}10]$ or $[\bar{2}\bar{1}0]$	6 on the 1st VD
cubic	[100] or [010] or [001]	[111] or $[1\bar{1}\bar{1}]$ or $[\bar{1}1\bar{1}]$ or $[\bar{1}\bar{1}1]$	[110] or [011] or [101] or $[1\bar{1}0]$ or $[10\bar{1}]$ or $[01\bar{1}]$	3 on the 2nd VD

Wyckoff Positions

- Wyckoff positions are used to efficiently place atoms or molecules in the lattice.
- A Wyckoff position is any point in a set of points whose site symmetry groups are all conjugate subgroups one of another.

Literature Research on Space Groups and Wykoff Positions

- The International Tables for Crystallography collect relevant theoretical data to all space groups.
- An example might be space group 225 which is relevant for the Cu prototype:



http://it.iucr.org/A/

Literature Research on Space Groups and Wykoff Positions

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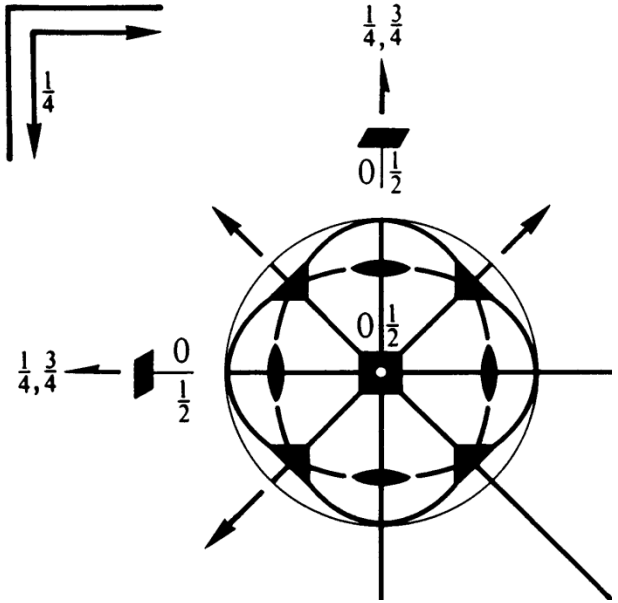
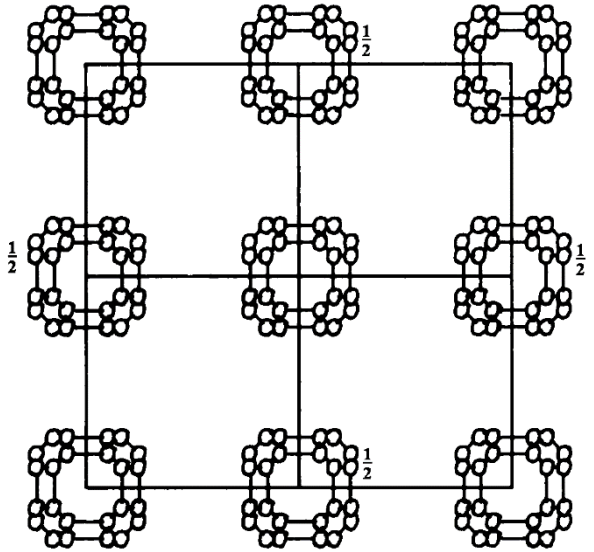
Depiction of the position of the symmetry elements
(triangle = threefold axis,
ellipse = twofold axis,
square = fourfold axis,
tails indicate screw axes, etc.)



Depiction of the general position



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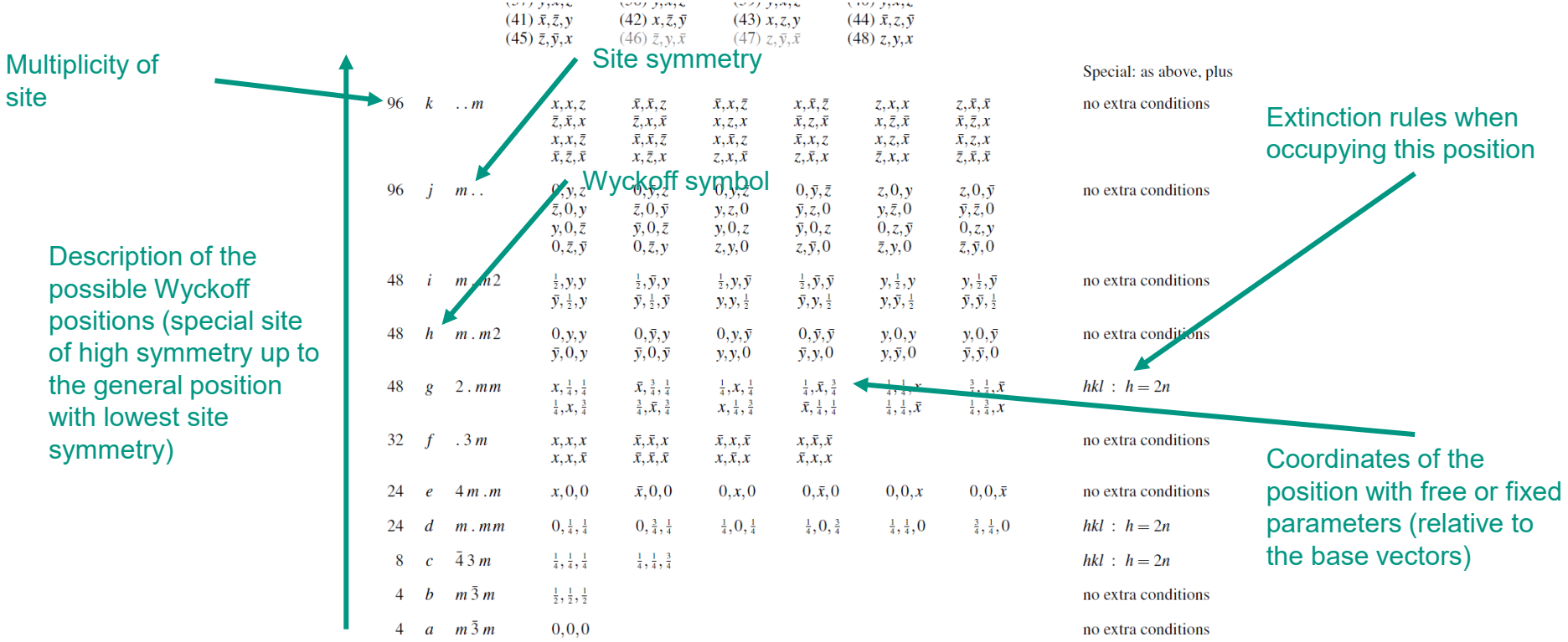
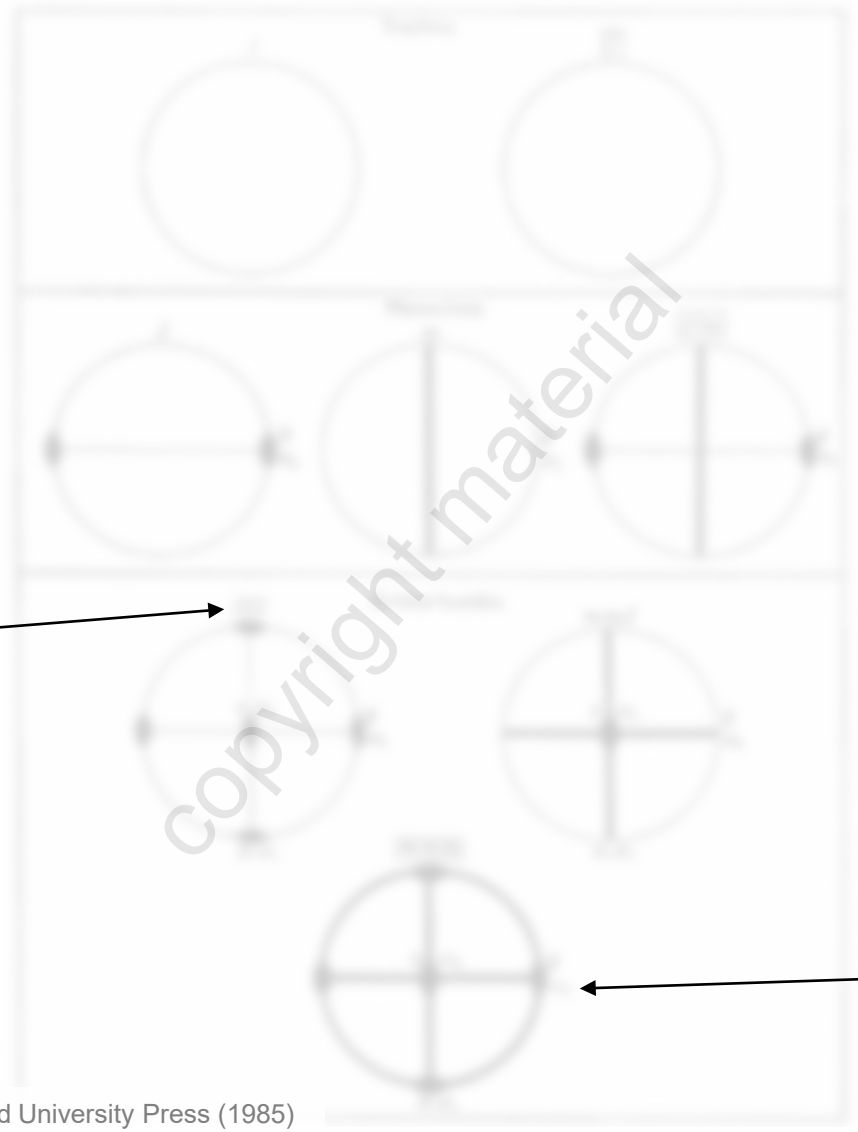


http://it.iucr.org/A/

Application



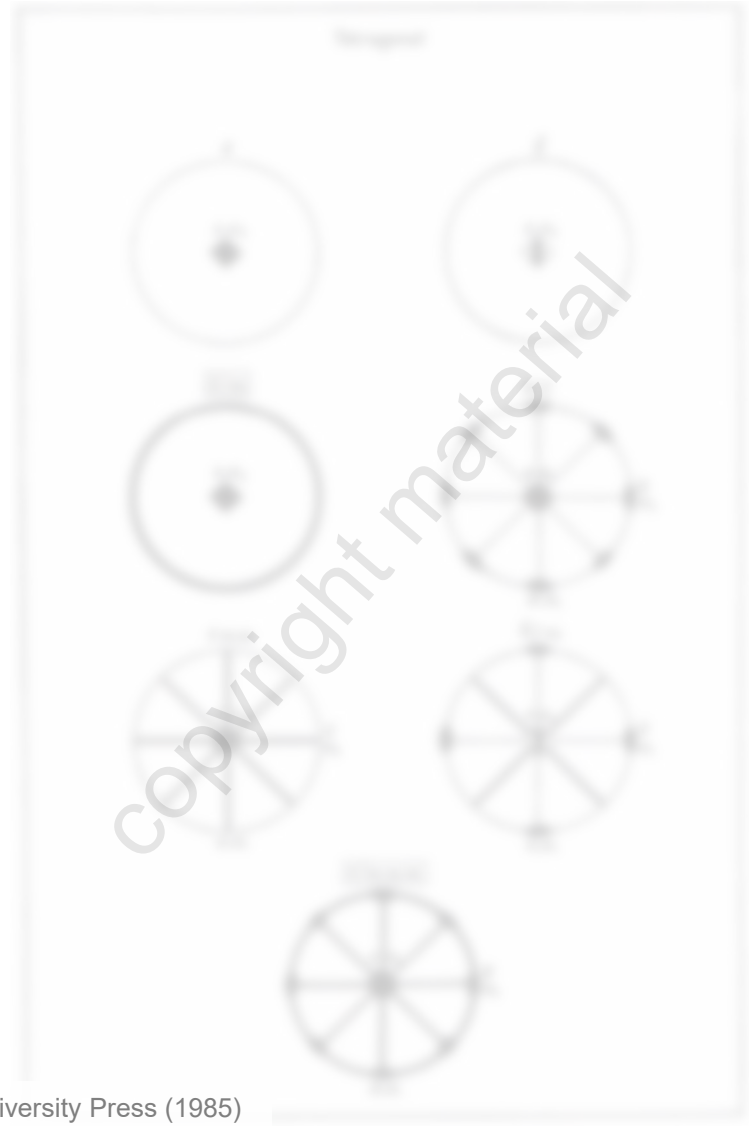
triclinic
only 1 or $\bar{1}$

monoclinic
only 2 or m

orthorhombic
only 2 or m along all principle axes

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

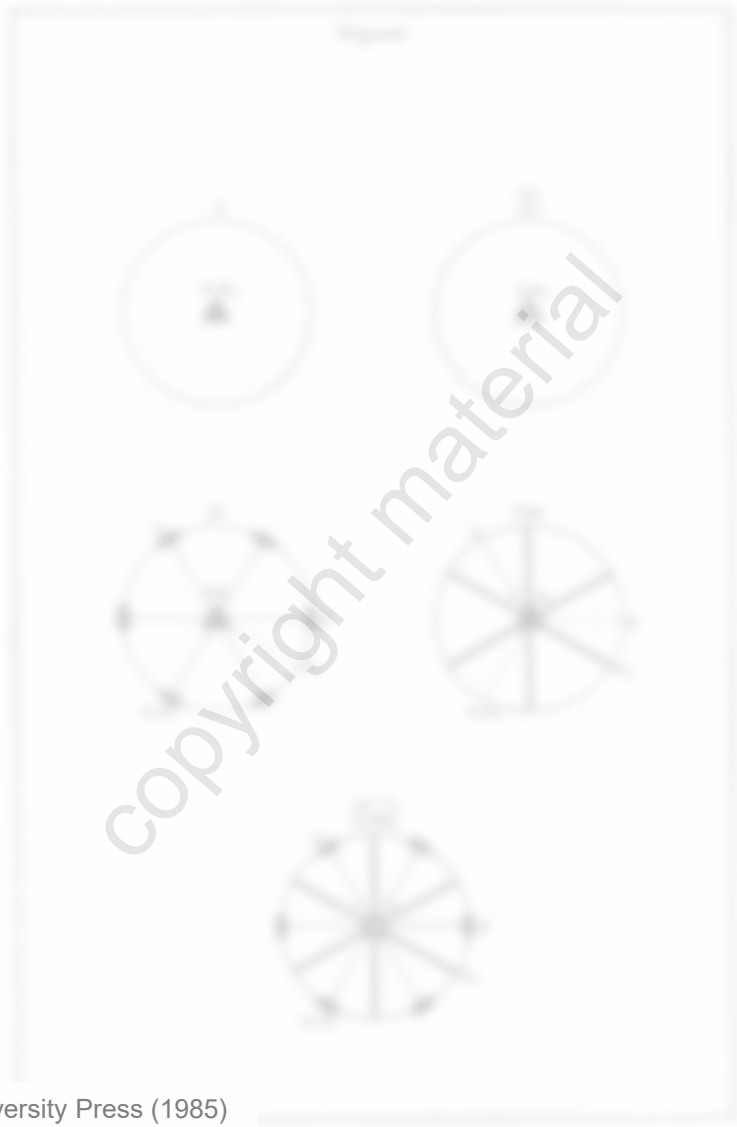
Application



tetragonal
always 4 or $\bar{4}$ along the axis of anisotropy

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

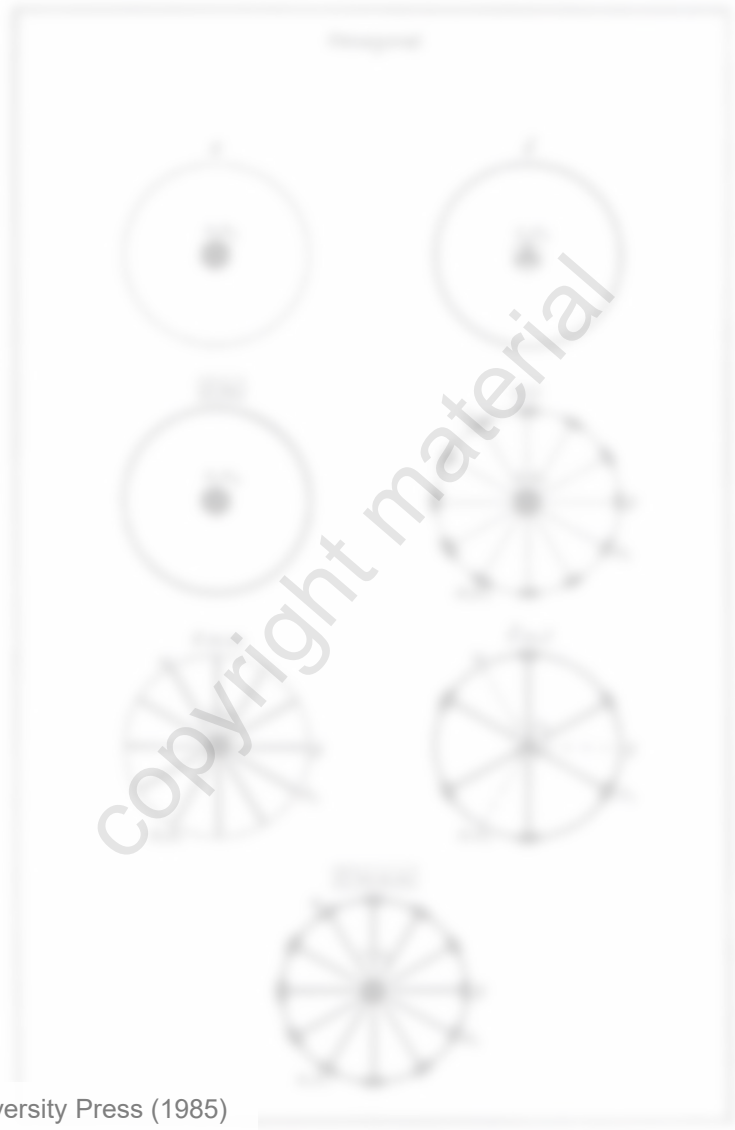
Application



trigonal
always 3 or $\bar{3}$ along the space diagonals

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

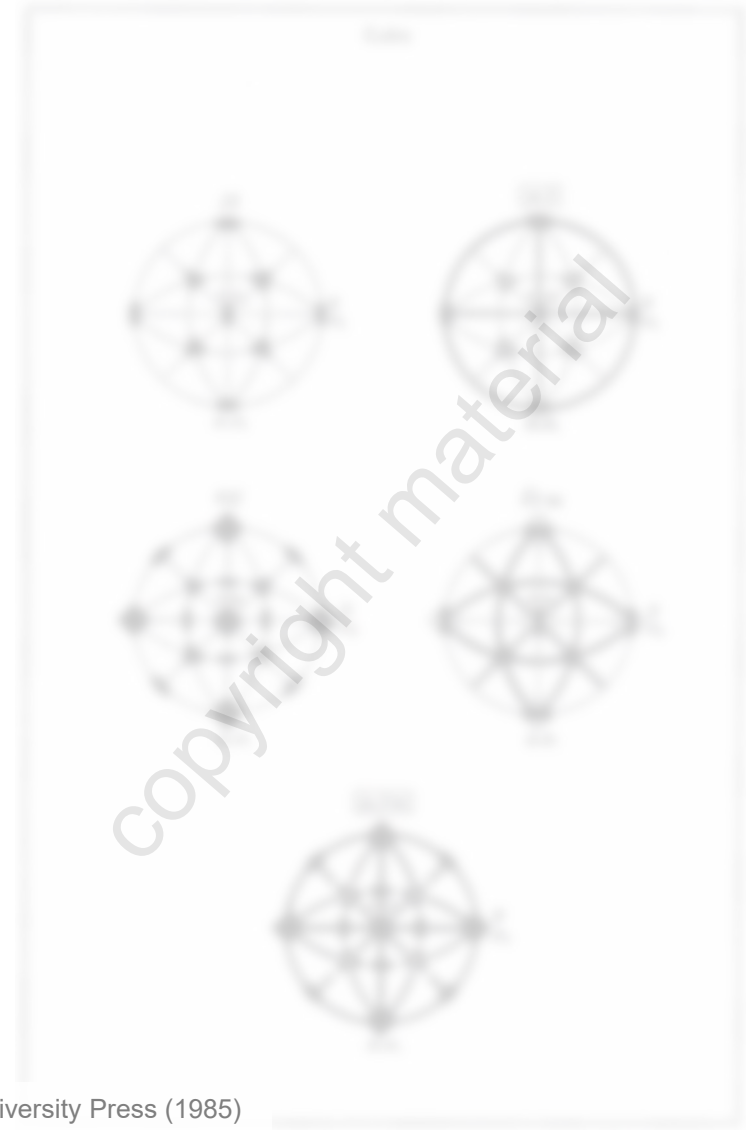
Application



hexagonal
always 6 or $\bar{6}$ along the axis of anisotropy

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application



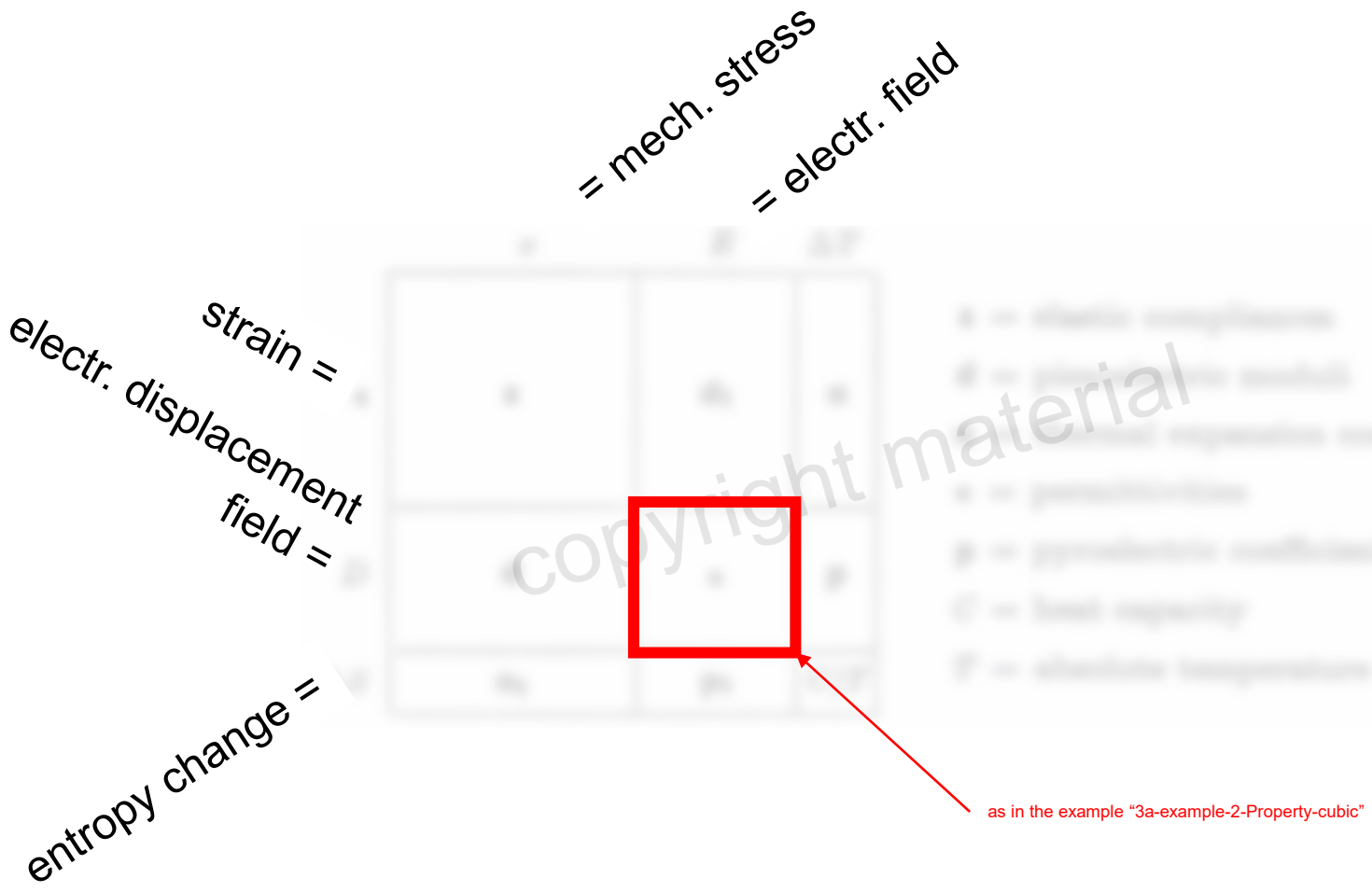
cubic
always 3 or $\bar{3}$ along the space diagonals

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application

- Similar to the example, the independent and dependent components of tensor property of materials can then be determined.
- They are typically visualized as follows; for easy representation in Voigt notation.

Application



J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application

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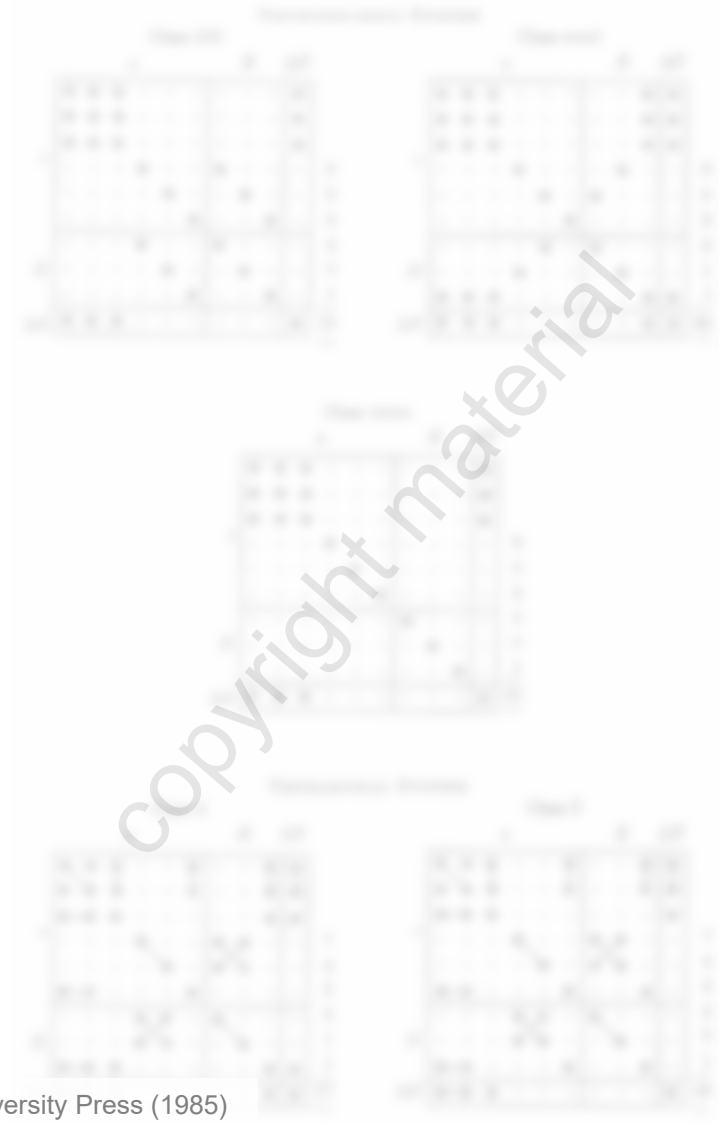
Application

triclinic

monoclinic

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application

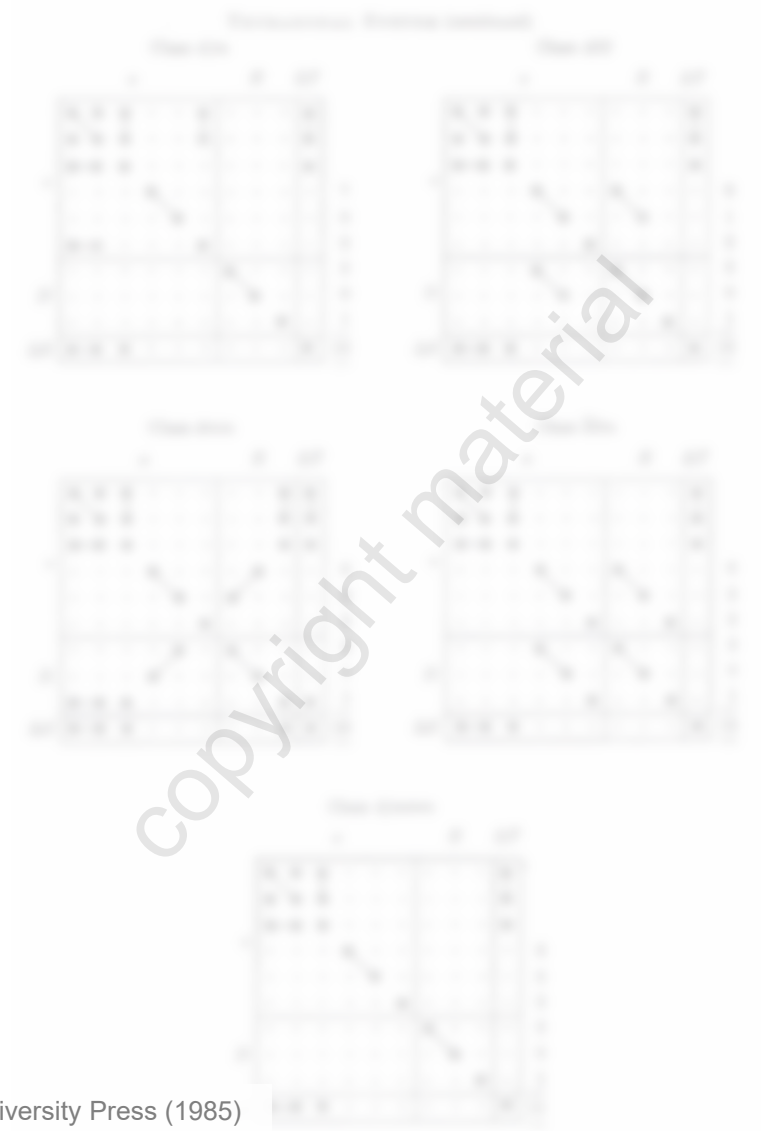


orthorhombic

tetragonal

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

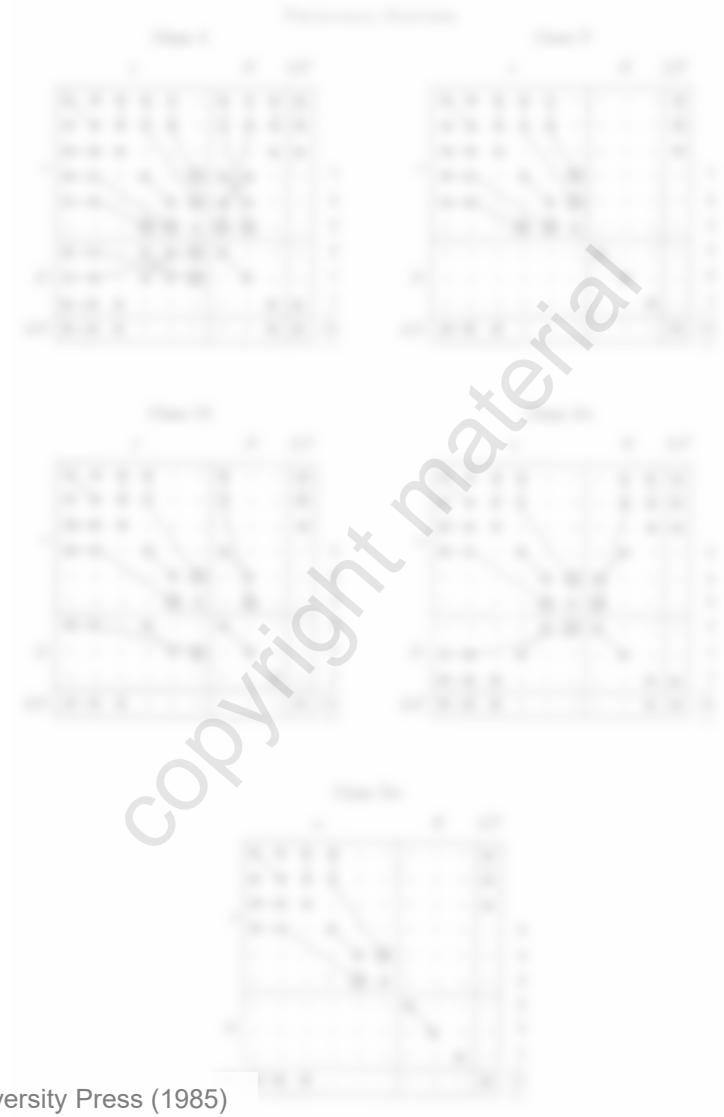
Application



J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application

trigonal



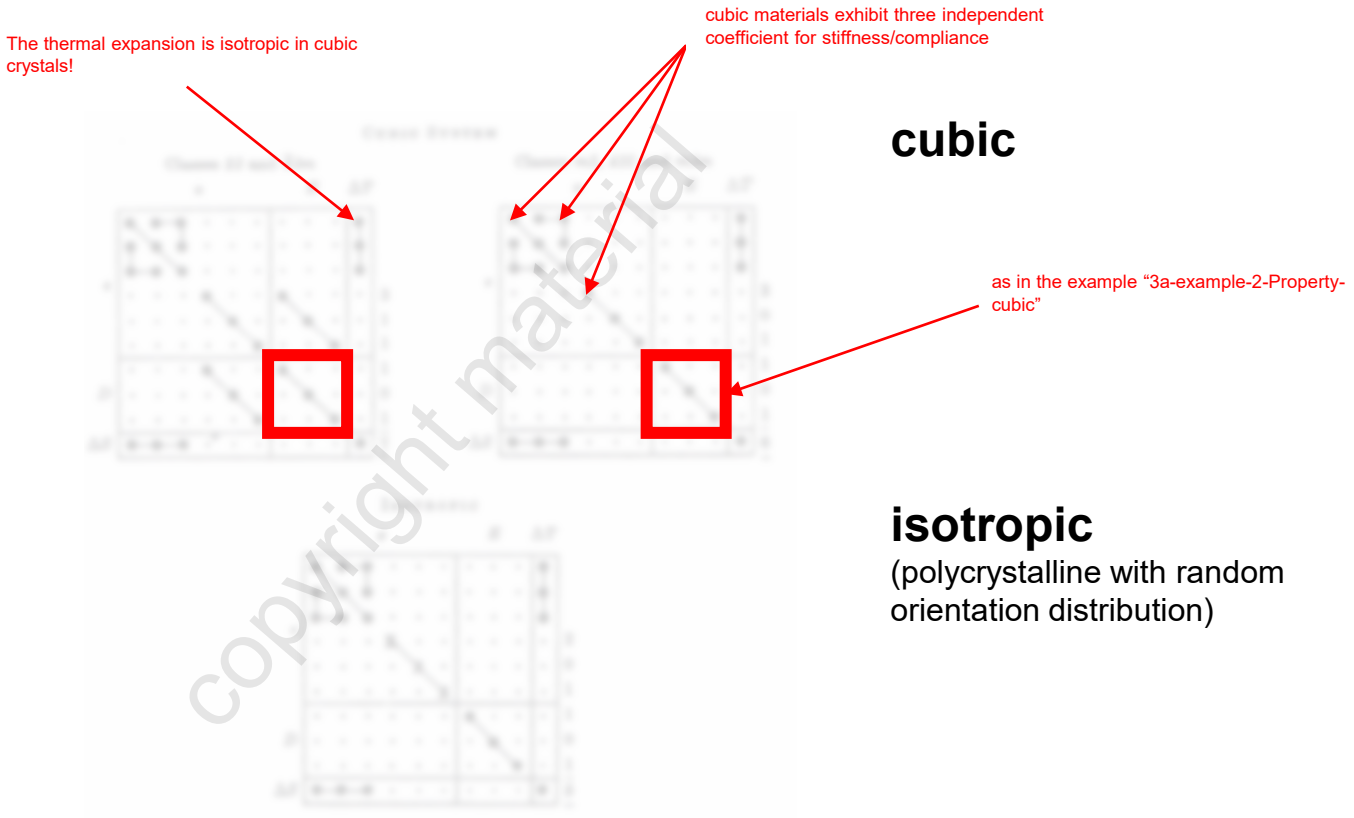
J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application

hexagonal

J. F. Nye: “Physical Properties of Crystals”, New York: Oxford University Press (1985)

Application



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