Symmetry

Read

Ott Chapter 6; 10.1

Sherwood & Cooper Chapter 3.1 ~ 3.7

Hammond Chapter 2.1 ~ 2.3; 12.5.1; 12.5.2

Krawitz Chapter 1.1 ~ 1.3

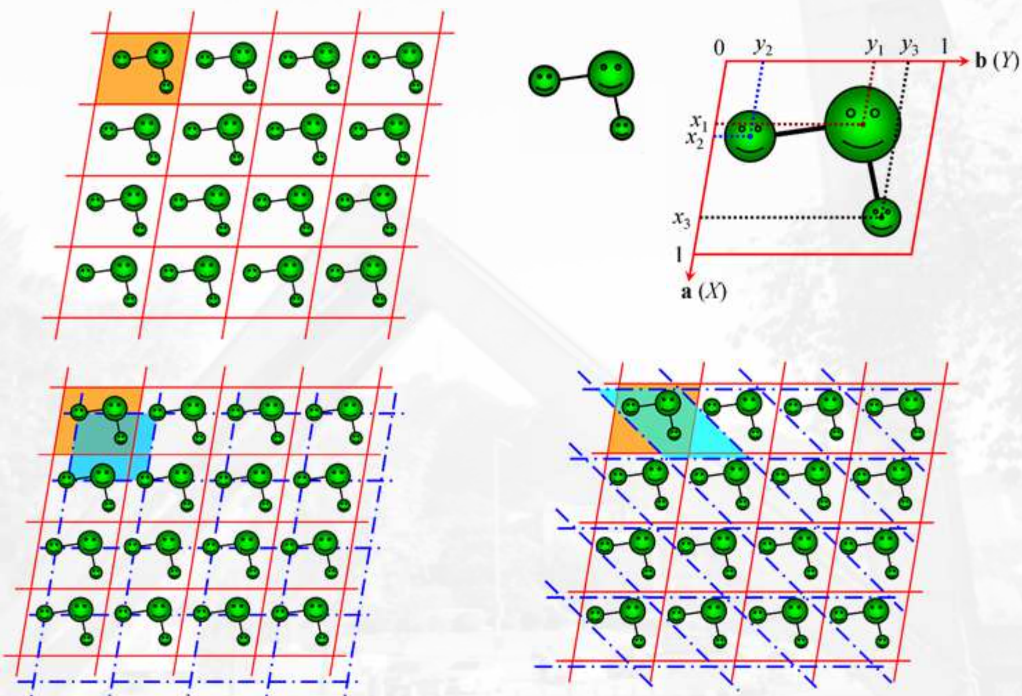
Use

http://materials.cmu.edu/degraef/pg/pg_gif.html

http://neon.mems.cmu.edu/degraef/pg/pg.html#AGM

Unit cell

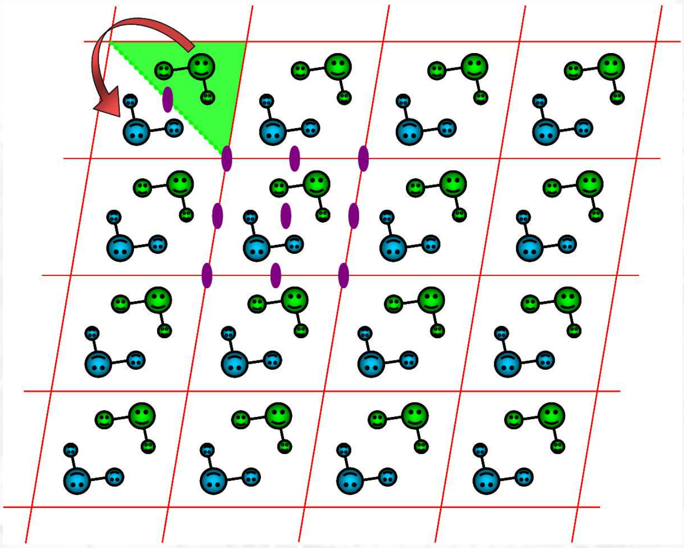
- the smallest unit of volume that contains all of the structural and symmetry information and that can reproduce a pattern in all of space by translation.



Pecharsky Chap 1

Asymmetric unit

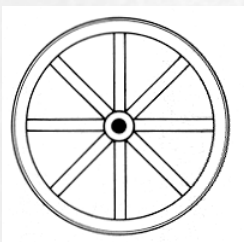
- the smallest part of the unit cell from which the whole cell can be filled exactly by the operation of all the symmetry operations
- the smallest unit of volume that contains all the structural information and that can reproduce the unit cell by application of the symmetry operations.

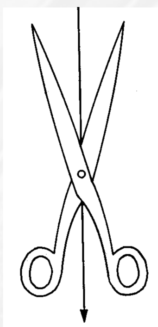


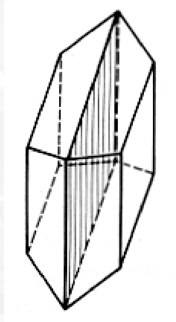
Pecharsky Chap 2

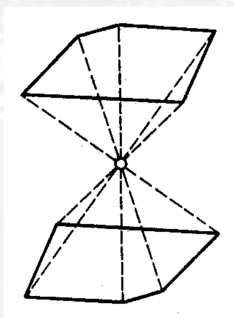
Symmetry

- Repetition operation = symmetry operation
  - ✓ Translation
    - Three non-coplanar lattice translation → space lattice
  - ✓ Rotation (회전)
  - ✓ Reflection (반사)
  - ✓ Inversion (반전)



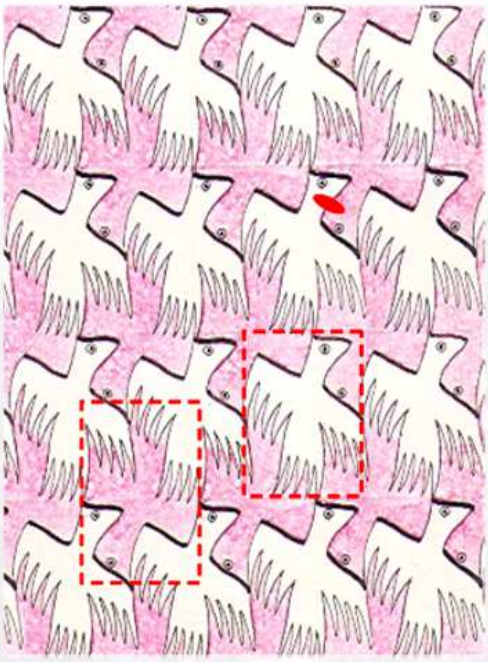






Ott Chap 6

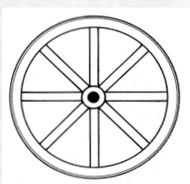
Unit cell & symmetry



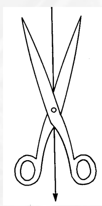
Symmetry

- All repetition operations are called <u>**symmetry operations**</u>
  - ✓Symmetry consists of the <u>repetition of a pattern</u> by the application of <u>specific rules</u>
- When a symmetry operation has a locus (a point, a line, or a plane) that is left unchanged by the operation, this locus is referred to as the <u>**symmetry element**</u>

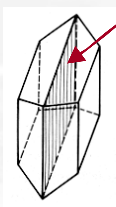
Symmetry operation	Geometrical representation	Symmetry element
Rotation	Axis (line)	Rotation axis
Inversion	Point (center)	Inversion center (center of symmetry)
Reflection	Plane	Mirror plane
Translation	vector	Translation vector



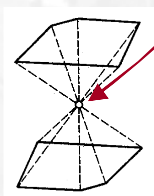
rotation



rotation



reflection



inversion

Ott Chap 6

Symmetry operation

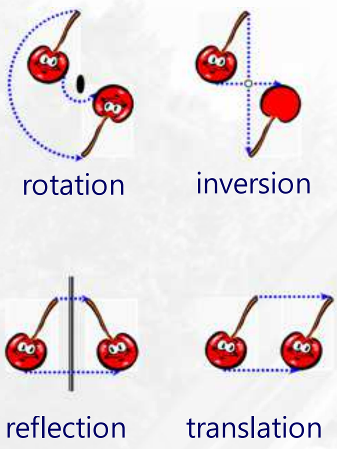
(1) Rotation; **1 2 3 4 6** (2) Reflection; **m** (= $\bar{2}$)

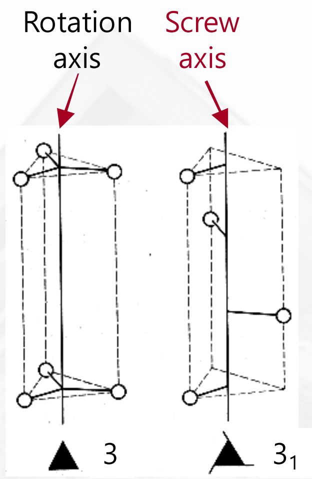
(3) Inversion (center of symmetry) (= $\bar{1}$)

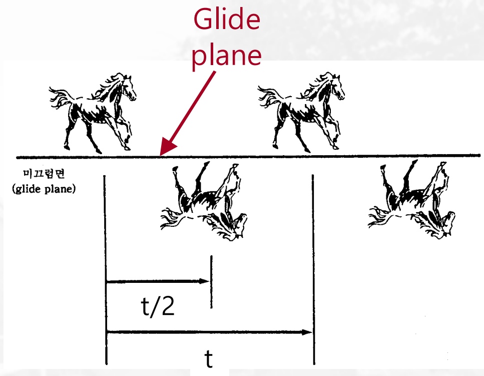
(4) Rotation-inversion; $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$

(5) Screw axis; rotation + translation **2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1,---, 6_5**

(6) Glide plane; reflection + translation, **a, b, c, n, d**



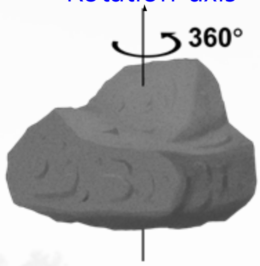




Ott Chap 10
Pecharsky Chap 2, 3

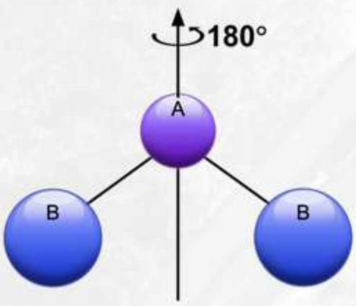
Symmetry

360°
Rotation axis

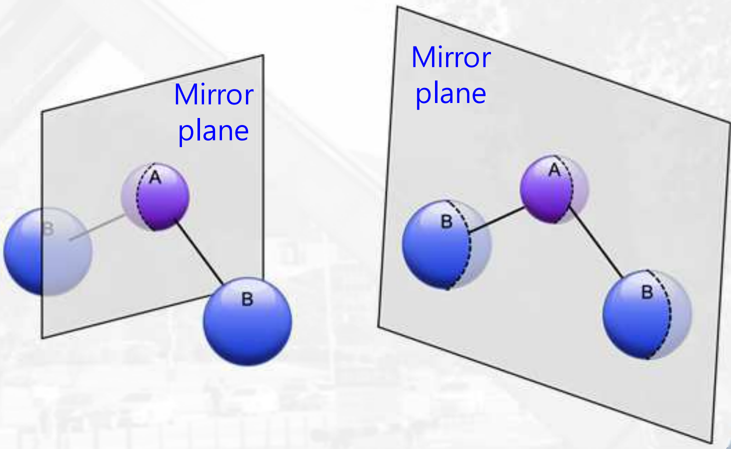


360°
Rotation
axis

180°
Rotation axis



Molecule AB_2



Point symmetry operation (without translation)

International notation (Hermann-Mauguin notation)

1, 2, 3, 4, 6, $\bar{1}$, $\bar{2}$(m), $\bar{3}$, $\bar{4}$, $\bar{6}$

Schoenflies notation

$\mathbf{C_1}$ = 1, $\mathbf{C_2}$ = 2, $\mathbf{C_3}$ = 3, $\mathbf{C_4}$ = 4, $\mathbf{C_6}$ = 6

$\mathbf{C_i(S_2)}$ = $\bar{1}$, $\mathbf{C_s}$ = $\bar{2}$(m), $\mathbf{C_{3i}(S_6)}$ = $\bar{3}$, $\mathbf{S_4}$ = $\bar{4}$, $\mathbf{C_{3h}}$ = $\bar{6}$

Rotation axis

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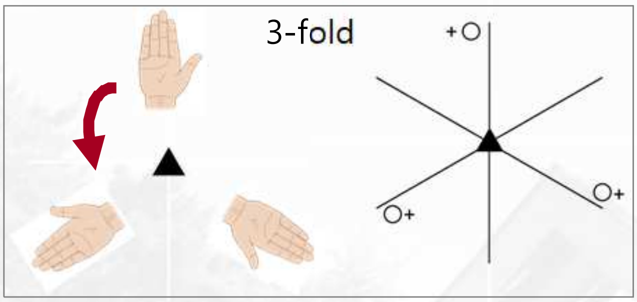
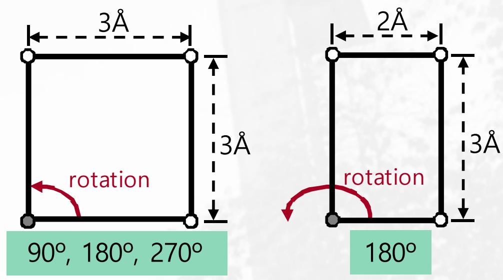
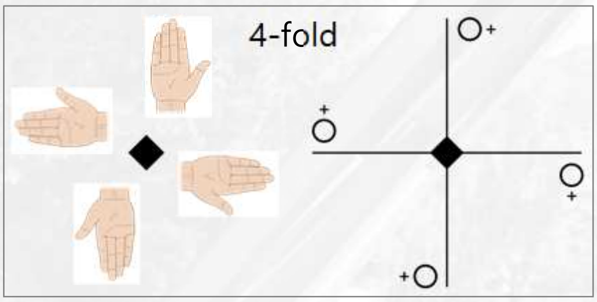
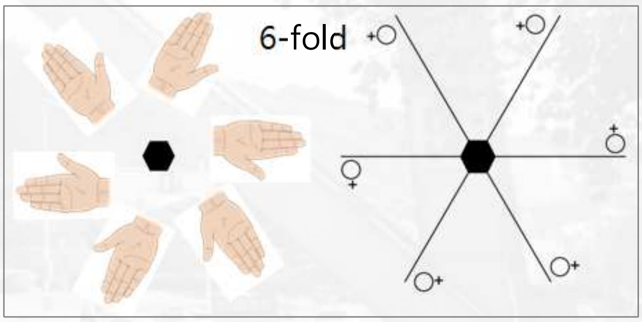
- n-fold axis $n = \dfrac{360^o}{\phi} = \dfrac{2\pi}{\phi}$ ϕ: minimum angle required to reach a position indistinguishable from the starting point





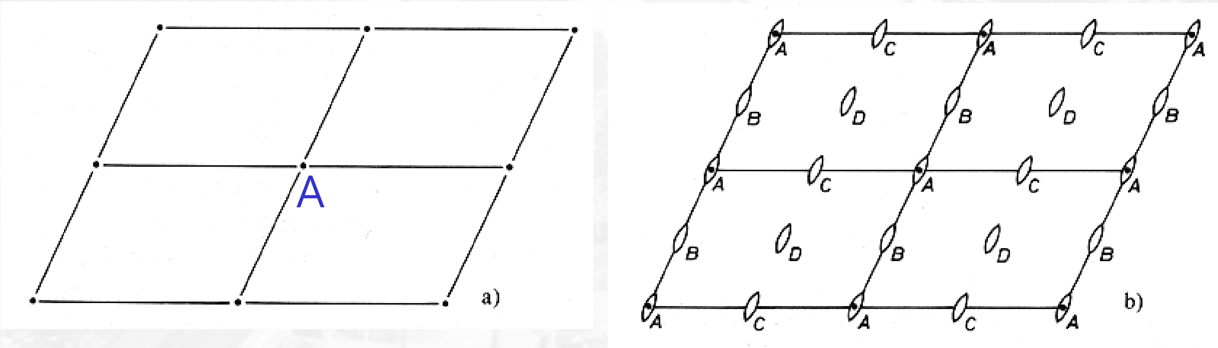




Rotation axis

- general plane lattice
- 180° rotation about the central lattice point A → coincidence
- A symbol for 2-fold rotation axis: digit 2
  - ✓ if it is ⊥ to the plane of the paper
  - ✓ → if it is // to the plane of the paper

Order (multiplicity) of the rotation axis, $n = \dfrac{360^{o}}{\phi} = \dfrac{2\pi}{\phi}$

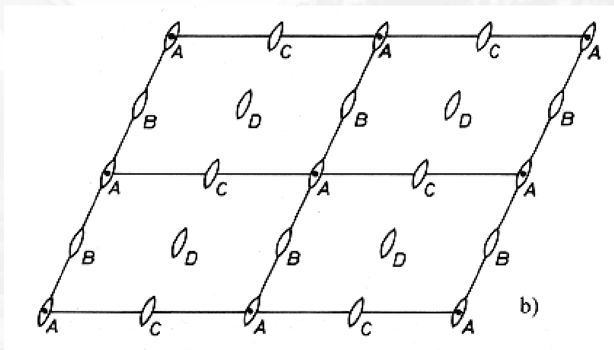


Equivalent vs. Identical

- Two objects are **EQUIVALENT**
  - ✓ When they can be brought into coincidence by application of a symmetry operation.
- Two objects are **IDENTICAL**
  - ✓ When no symmetry operation except lattice translation is involved.
  - ✓ equivalent by translation

- All A's are equivalent to one another.
- All B's are equivalent to one another.

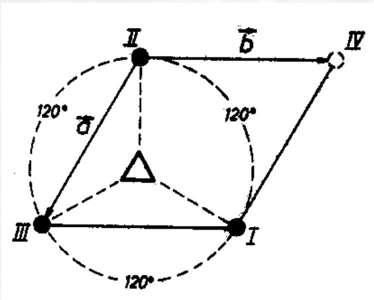
- A is not equivalent to B.



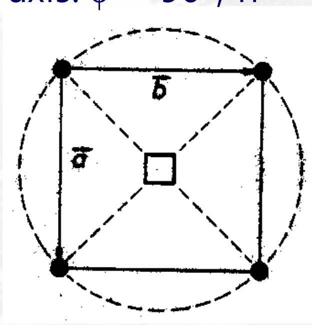
Rotation axis

- n-fold axis $n = \frac{360^o}{\phi} = \frac{2\pi}{\phi}$ ϕ: minimum angle required to reach a position indistinguishable from the starting point
- Axis with n > 2 will have at least two other points lying in a plane normal to it.
  - ✓ 3 non-colinear points define a plane → **must be a lattice plane** (translational periodicity)

3-fold axis: ϕ = 120º, n = 3 ▲



4-fold axis: ϕ = 90º, n = 4 ■



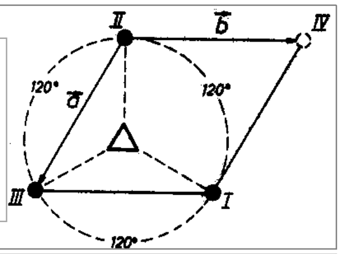
To be a lattice plane

- The points generated by rotation axis must fulfil the **conditions for being a lattice plane** --- parallel lattice lines should have the same translation period (all the lattice points should have identical surroundings)

3-fold rotation axis

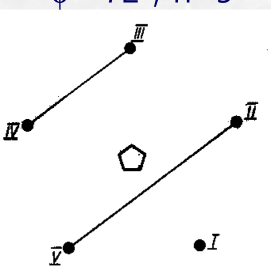
- Lattice translation moves I → IV
- 4 points produce a unit mesh of a lattice plane

→ 3 fold axes are compatible with space lattice



No 5-fold rotation axis in space lattice

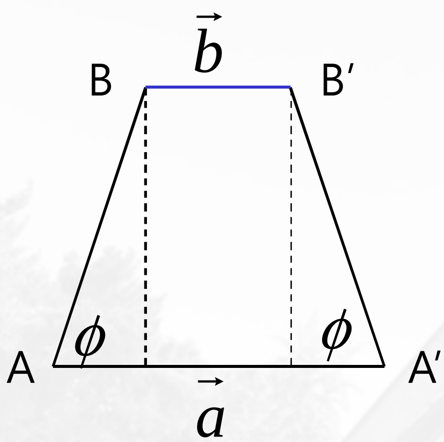
ϕ= 72º, n=5



- II-V and III-IV parallel but not equal or integral ratio
  → no 5-fold axes in space lattice
- This structure does not have translational symmetry in 3-dimensions
  → do not have finite unit cell → quasicrystal
  - ✓ Quasi – because there is no translational symmetry
  - ✓ Crystal – because they produce discrete, crystal-like diffraction patterns
- It is impossible to completely fill the area in 2-dimensions with pentagons without creating gaps

- a. almost, near, partially, partly, somewhat, ersatz, imitation, pseudo, synthetic, apparent, seeming, supposed
- '유사(類似), 의사(擬似), 준(準)' 등의 뜻: quasi-cholera (유사 콜레라), a quasiwar (준전쟁).
- 의사(擬似) - false; suspected; para-.

- limitation of ϕ set by **translation periodicity**



$\vec{b} = m\vec{a}$ where m is an integer

$$ma = a - 2a\cos\phi$$

$$m = 1 - 2\cos\phi$$

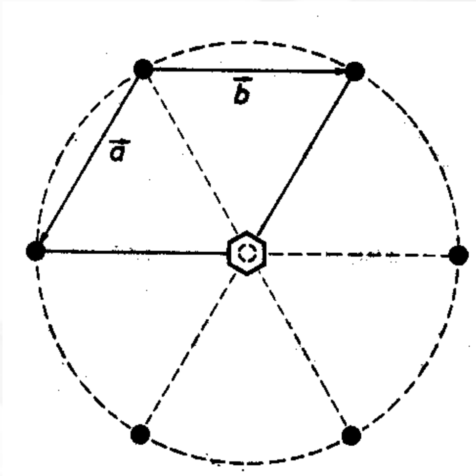
$$\cos\phi = \frac{1-m}{2}$$

m	cos ϕ	ϕ	n
-1	1	2π	**1**
0	½	π/3	**6**
1	0	π/2	**4**
2	- ½	2π/3	**3**
3	-1	π	**2**

See Sherwood & Cooper page 78

Rotation axis

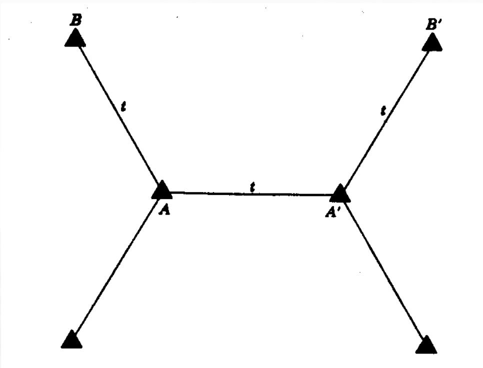
6-fold axis: ϕ=60^{o}, n=6

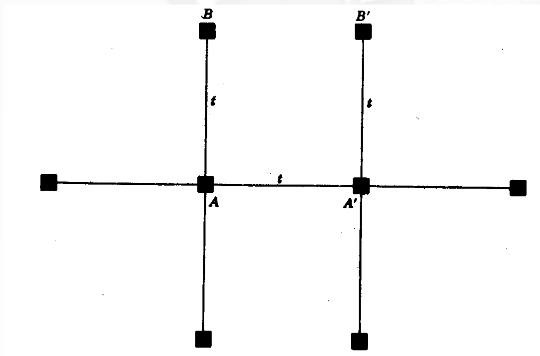


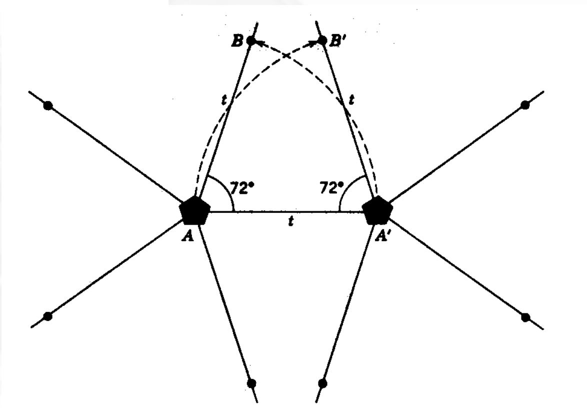
- In space lattices and consequently in crystals, only 1-, 2-, 3-, 4-, and 6-fold rotation axes can occur.

Ott Chap 6

Rotation axis







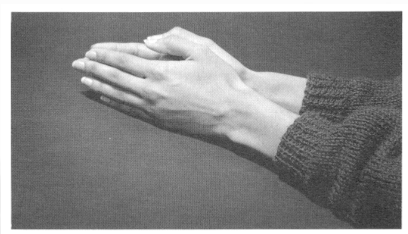
Symmetry operation vs Symmetry element, Proper vs Improper

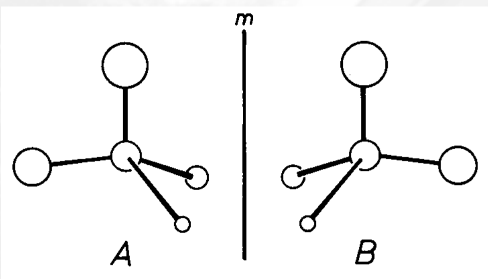
- Rotation by 60° around an axis → **symmetry operation**
- 6-fold rotation axis is a **symmetry element** which contains six rotational symmetry operations

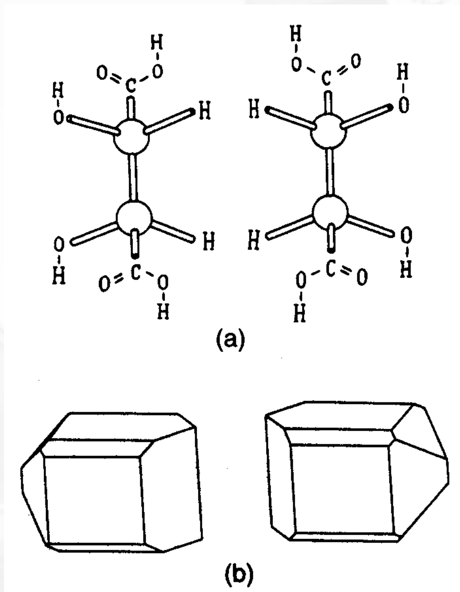
- **Proper** symmetry elements
  - ✓Rotation axes, screw axes, translation vectors
- **Improper** symmetry elements
  - ✓Inverts an object in a way that may be imaged by comparing right & left hands
  - ✓Inverted object is called an **enantiomorph** of the direct object (right vs left hand)
  - ✓Center of inversion, roto-inversion axes, mirror plane, glide plane

Reflection

- a plane of symmetry or a mirror plane, m, **| (bold line)**



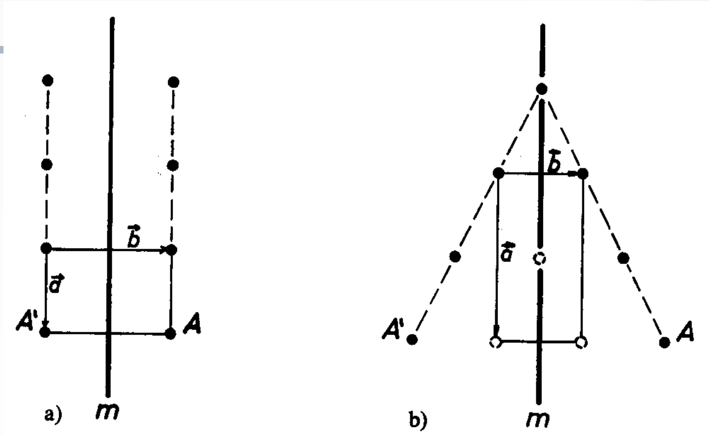




Ott Chap 6
Hammond Chap 4

Reflection

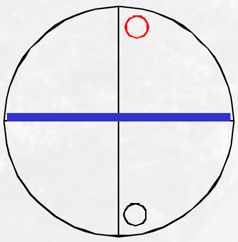
Lattice line // m



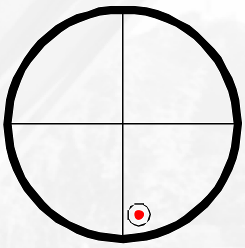
Lattice line tilted w.r.t. m

rectangular

centered rectangular



m_{yz} (m_x)



m_{xy} (m_z)

● down

○ up

Black & Red; enantiomorphs

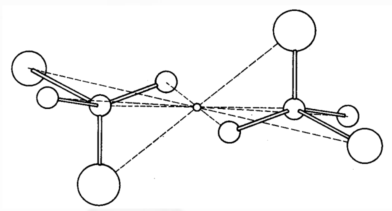
● down, left-hand

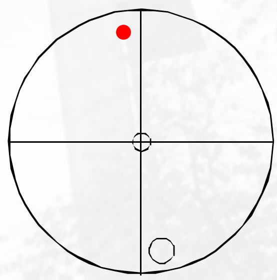
○ up, right-hand

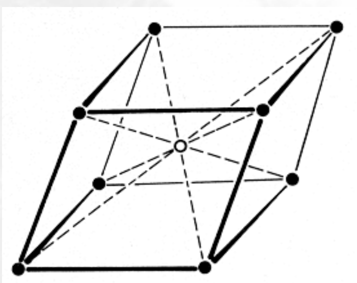
Ott Chap 6

Inversion

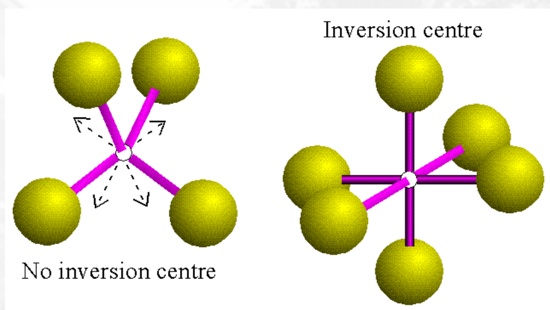
- center of symmetry or inversion center, ○ $\bar{1}$
- centrosymmetric







All lattices are centrosymmteric



http://www.gh.wits.ac.za/craig/diagrams/

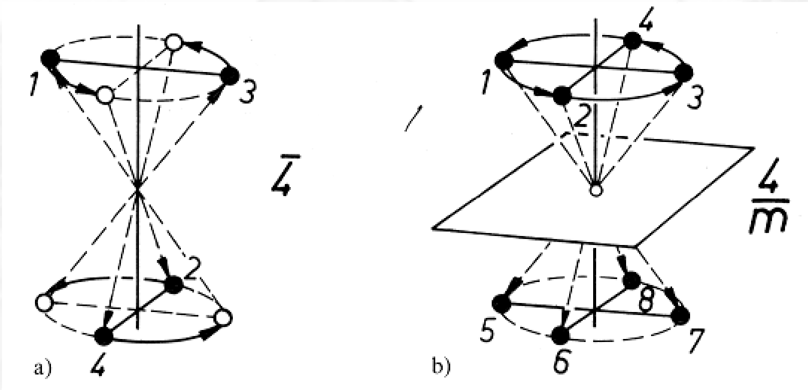
Ott Chap 6
Hammond Chap 4

Compound symmetry operation

- link of translation, rotation, reflection, and inversion operation
- compound symmetry operation
  - ✓ two symmetry operation in sequence as a single event
- combination of symmetry operations
  - ✓ two or more individual symmetry operations are combined, which are themselves symmetry operations

$4 + \bar{1}$

4 & $\bar{1}$ are not present



$4 + \bar{1}$

4 & $\bar{1}$ are present

compound combination

Compound symmetry operation

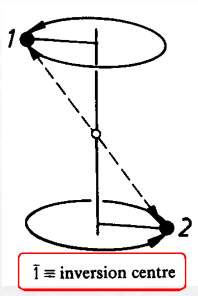
Table 5.1. Compound symmetry operations of simple operations. The corresponding symmetry elements are given in round brackets

	Rotation	Reflection	Inversion	Translation
Rotation	×	Roto-reflection	Roto-inversion	Screw rotation
Reflection	(Roto-reflection axis)	×	2-fold rotation	Glide reflection
Inversion	(Roto-inversion axis)	(2-fold rotation axis)	×	Inversion
Translation	(Screw axis)	(Glide plane)	(Inversion centre)	×

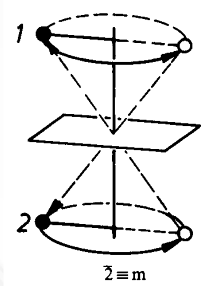
Rotoinversion

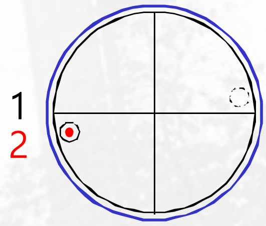
- compound symmetry operation of rotation and inversion
- rotoinversion axis $\bar{n}$
- 1, 2, 3, 4, 6 → $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$

$\boxed{\bar{1}}$

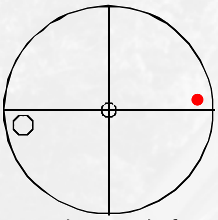


$\boxed{\bar{2}(\equiv m)}$





m_{xy} (m_z)

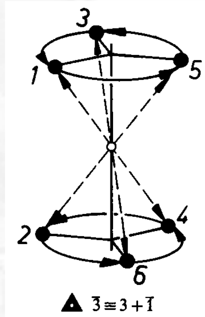


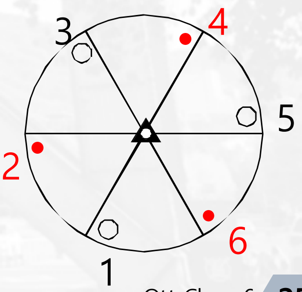
● down, left

○ up, right

$\boxed{\bar{3} \equiv 3 + \bar{1}}$

Rare case of "compound symmetry operation = combination of symmetry operation"



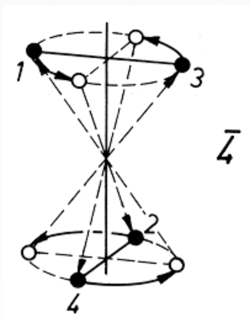


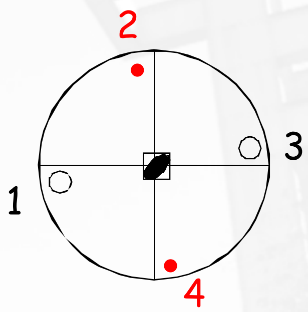
Ott Chap 6

Rotoinversion

$\bar{4}$

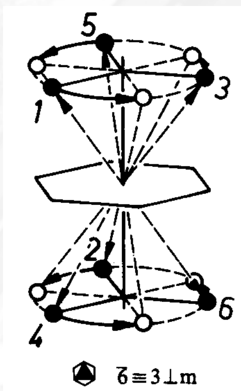
$\bar{4}$ implies the presence of a parallel 2

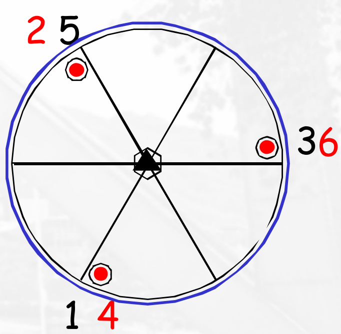




$\bar{6}$

$\boxed{\bar{6} \equiv 3 \perp m}$



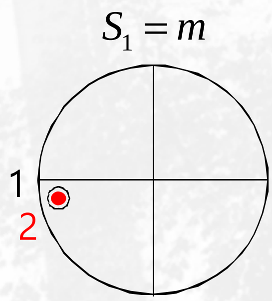


Ott Chap 6

Rotoinversion & Rotoreflection

Rotoinversion

- $\bar{1}$ ≡ inversion center, $\bar{2}$ ≡ m, $\bar{3}$ ≡ 3 + $\bar{1}$, $\bar{4}$, $\bar{6}$ ≡ 3 ⊥ m
- only rotoinversion axes of odd order ($\bar{1}$, $\bar{3}$) have an inversion center



Rotoreflection

$$S_1 = m \quad S_2 = \bar{1} \quad S_3 = \bar{6} \quad S_4 = \bar{4} \quad S_6 = \bar{3}$$

- The axes n and $\bar{n}$, including $\bar{1}$ and m, are called **point-symmetry elements**, since their operations always leave at least one point unmoved.

Ott page 71; $\bar{4}$ implies the presence of a parallel 2.

Symmetry elements, Proper vs Improper

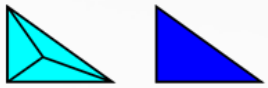
- 1, 2, 3, 4, 6 --- proper rotation axes
- $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$ --- improper rotation axes; right & left hands → enantiomorph
- Screw axes (rotation + translation) 2_1 3_1 3_2 4_1 4_2 4_3 6_1 6_2 6_3 6_4 6_5
- Glide planes (reflection + translation) a b c n d

Translation symmetry is not included in 1, 2, 3, 4, 6, $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$, and $\bar{6}$.

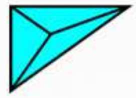
- Proper symmetry elements
  - ✓Rotation axes, screw axes, translation vectors
- Improper symmetry elements
  - ✓Inverts an object in a way that may be imaged by comparing right & left hands
  - ✓Inverted object is called an **enantiomorph** of the direct object (right vs left hand)
  - ✓Center of inversion, roto-inversion axes, mirror plane, glide plane

Translation 병진
Mirror plane 거울면
Glide plane 영진면
Screw axes 나사축

Rotation axes

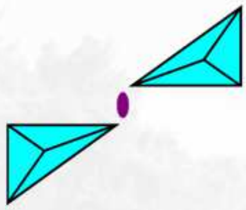


Enantiomorphous objects

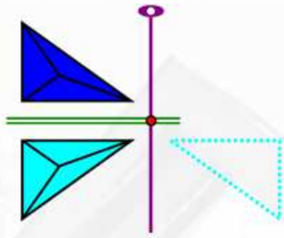


1-fold rotation axis

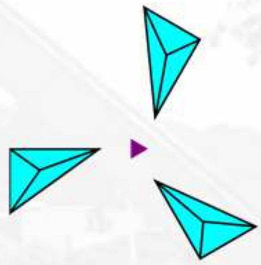
Center of inversion



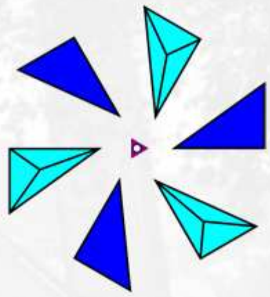
2-fold rotation axis



$\bar{2}$ = m



3-fold rotation axis



$\bar{3}$

Rotation axes

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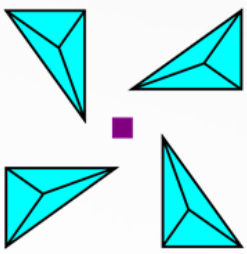
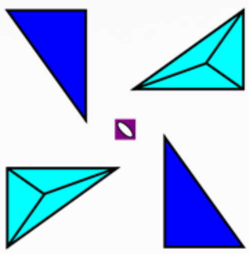
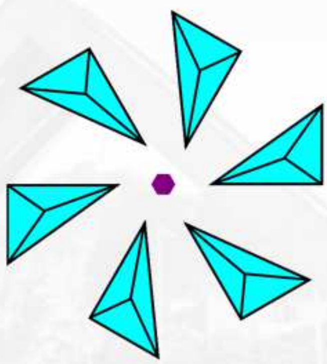


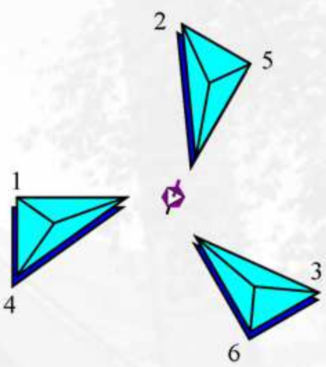
4-fold rotation axis



$\bar{4}$



6-fold rotation axis

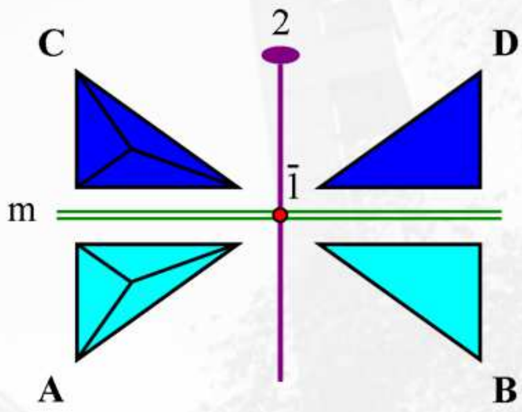


$\bar{6}$

Interaction of symmetry elements

Start with 2 and $\bar{1}$ (on 2) → m

New symmetry element "m" emerged as the result of the sequential application of two symmetry elements ("2" then "$\bar{1}$") to the original object.



2 X $\bar{1}$ (on 2) = $\bar{1}$ (on 2) X 2 = m (⊥ 2 thru $\bar{1}$)

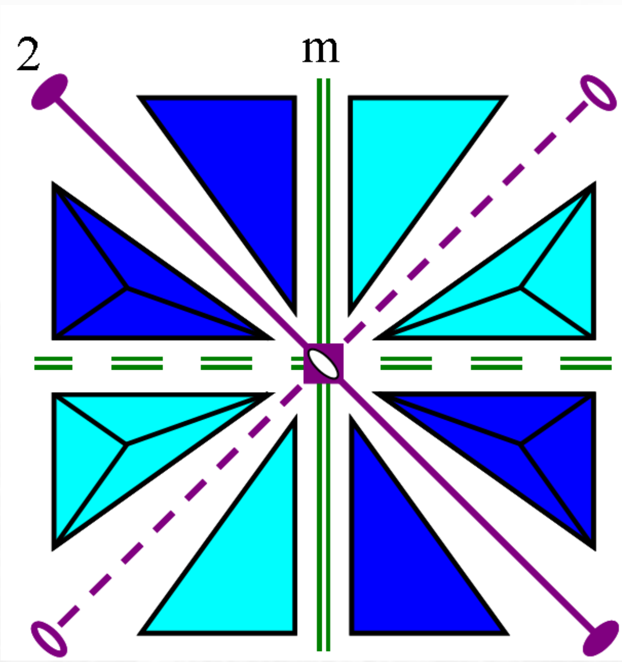
2 X m (⊥ 2) = m (⊥ 2) X 2 = $\bar{1}$ (@ m⊥ 2)

m X $\bar{1}$ (on m) = $\bar{1}$ (on m) X m = 2 (⊥ m thru $\bar{1}$)

When two symmetry elements interact, they result in additional symmetry element(s).

Interaction of symmetry elements

Start with 2 and m @45 degree angle → m, 2, $\bar{4}$



Symmetry group

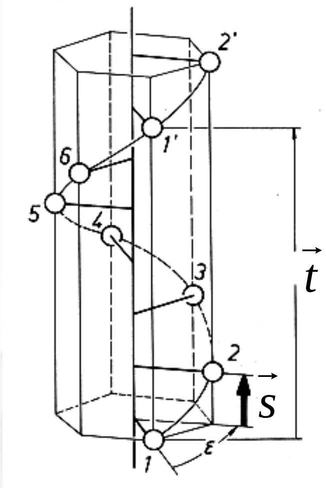
- Complete set of symmetry elements → symmetry group
- Limited # of symmetry elements (ten) & all valid combination among them → 32 crystallographic symmetry groups → 32 point groups
- Limited # of symmetry elements (ten) + the way in which they interact with each other → limited # of completed sets of symmetry elements (32 symmetry groups = 32 point groups)
- Point group ← symmetry elements in these groups have at least one common point and, as a result, they leave at least one point of an object unmoved.

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

7 crystal systems

- Combination of symmetry elements & their orientations w.r.t. one another defines the crystallographic axes.
- Axes can be chosen arbitrarily, but are usually chosen w.r.t. specific symmetry elements present in a group.
  - ✓ // rotation axes or ⊥ m
- All possible 3-D crystallographic point groups can be divided into a total of 7 crystal systems based on the presence of a specific symmetry elements or specific combination of them present in the point group symmetry.
- (7 crystal systems) X 5 (types of lattices) → 14 different types of unit cells are required to describe all lattices (14 Bravais lattices).

Screw axes
(rotation + translation)
나사축



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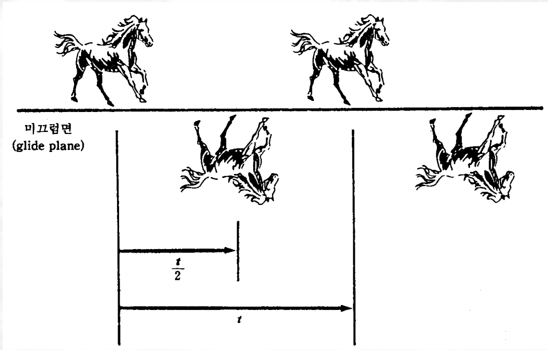
Glide planes
(reflection + translation)
영진면



New symmetry operations in centered Lattices

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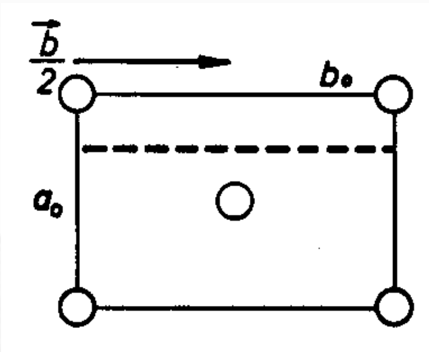
- orthorhombic C-lattice

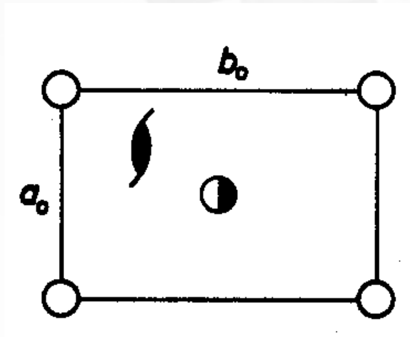


- reflection at $\frac{1}{4}, y, z$
  + translation $\frac{\vec{b}}{2}$

  $0,0,0 \;\rightarrow\; \frac{1}{2}, \frac{1}{2}, 0$

- glide reflection
- glide plane (b-glide)

- orthorhombic I-lattice



- rotation about $\frac{1}{4}, \frac{1}{4}, z$
  + translation $\frac{\vec{c}}{2}$

  $0,0,0 \;\rightarrow\; \frac{1}{2}, \frac{1}{2}, \frac{1}{2}$

- screw rotation
- screw axis (2_1-screw)

Compound symmetry operation

Table 5.1. Compound symmetry operations of simple operations. The corresponding symmetry elements are given in round brackets

	Rotation	Reflection	Inversion	Translation
Rotation	×	Roto-reflection	Roto-inversion	Screw rotation
Reflection	(Roto-reflection axis)	×	2-fold rotation	Glide reflection
Inversion	(Roto-inversion axis)	(2-fold rotation axis)	×	Inversion
Translation	(Screw axis)	(Glide plane)	(Inversion centre)	×

rotation + translation

reflection + translation

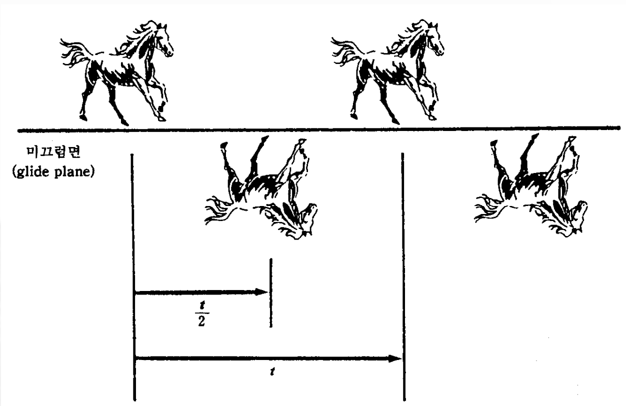
2-fold rotation + reflection

Glide plane

i) reflection

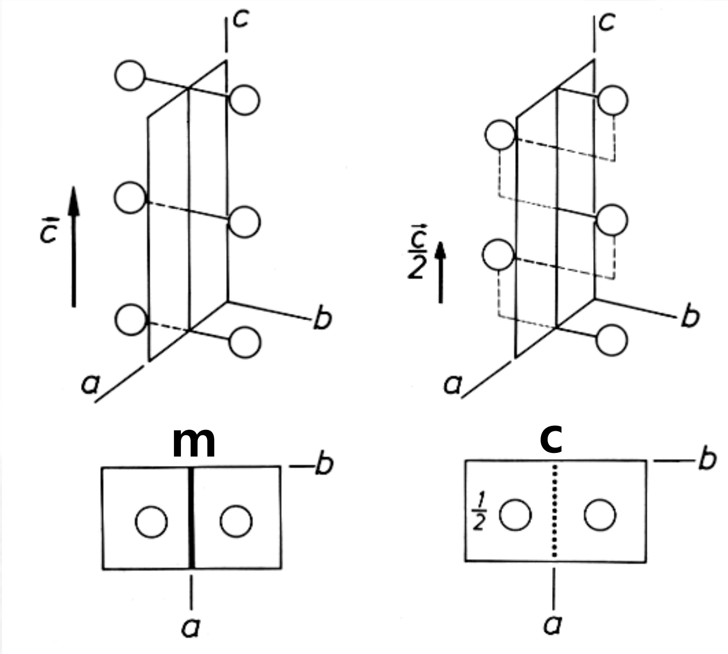
ii) translation by the vector $\vec{g}$ parallel to the plane of reflection

where $|\vec{g}|$ is called glide component



$\vec{g}$ is one half of a lattice translation parallel to the glide plane $\quad |\vec{g}| = \frac{1}{2}|\vec{t}|$

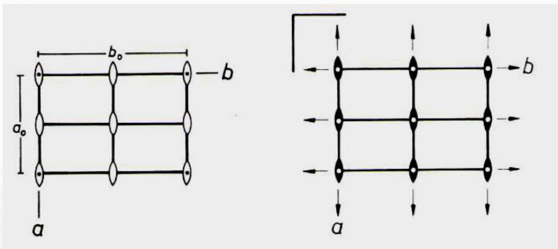
Mirror plane "m" vs. Glide plane "c"



- Glide plane can <u>only</u> occur in an orientation that is possible for a mirror plane.

Glide plane

Orthorhombic **P2/m2/m2/m**



a Plane lattice with rectangular unit mesh showing its symmetry. Stacking of such planes directly above one another with interplanar spacing c_0 leads to the orthorhombic P-lattice (cf. **b**)

d Space group

P 2/m 2/m 2/m (Pmmm)
↓ a ↓ b ↓ c

Projection of the symmetry elements of the orthorhombic P-lattice on x, y, 0. This is one of the space groups of highest symmetry in the orthorhombic system

b Orthorhombic P-lattice, lattice parameters in the unit cell are:

$a_0 \neq b_0 \neq c_0$
$\alpha = \beta = \gamma = 90°$

c Orthorhombic axial system

$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

Fig. 6.9a–f. The orthorhombic crystal system

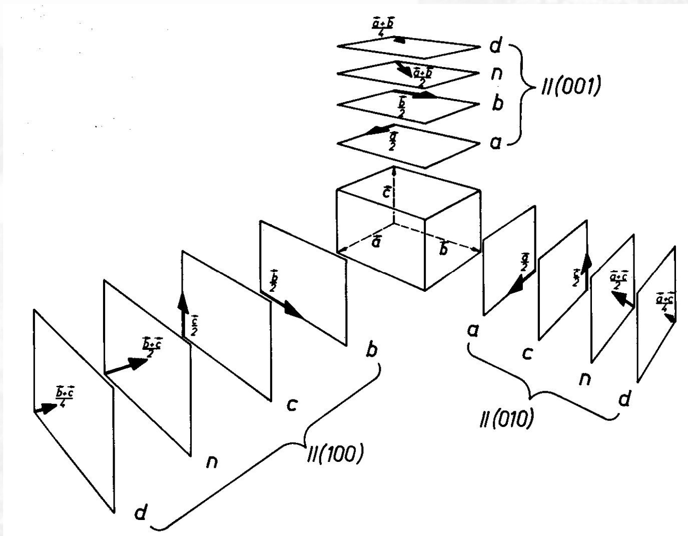
Ott Chap 7

Mirror planes along (100), (010), (001)

Glide plane // (100)

$$\rightarrow \frac{1}{2}\left|\vec{b}\right|,\ \frac{1}{2}\left|\vec{c}\right|,\ \frac{1}{2}\left|\vec{b}+\vec{c}\right|,\ \frac{1}{4}\left|\vec{b}\pm\vec{c}\right|$$

b-glide c-glide n-glide d-glide



Reflection plus ½ cell translation

- *a* - glide: *a*/2 translation
- *b* - glide: *b*/2 translation
- *c* - glide: *c*/2 translation
- *n* – glide (normal to *a*): *b*/2+*c*/2 translation
- *n* – glide (normal to *b*): *a*/2+*c*/2 translation
- *n* – glide (normal to *c*): *a*/2+*b*/2 translation
- *d* - glide : (*a* + *b*)/4, (*b* + *c*)/4, (*c* + *a*)/4
- <u>*g* - glide line (two dimensions)</u>

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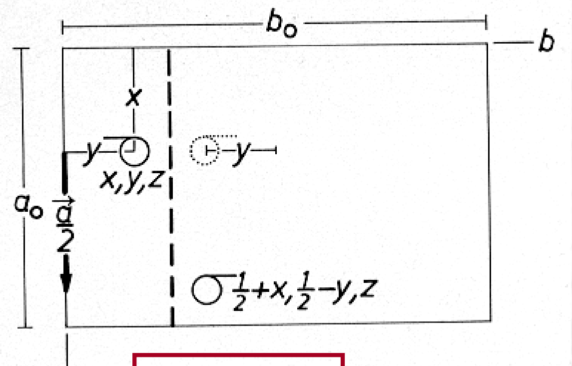
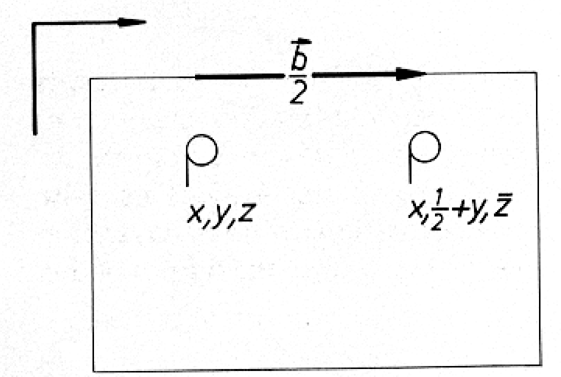
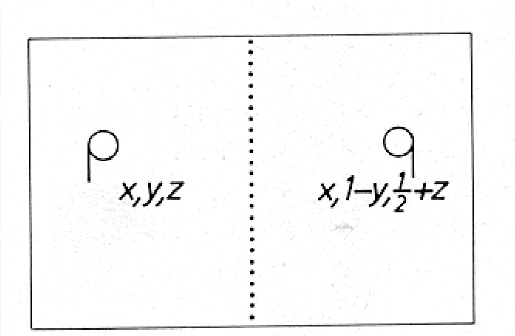
Orthorhombic cell
projected on x,y,o



a a-glide at x, $\frac{1}{4}$ z



b b-glide at x,y,0

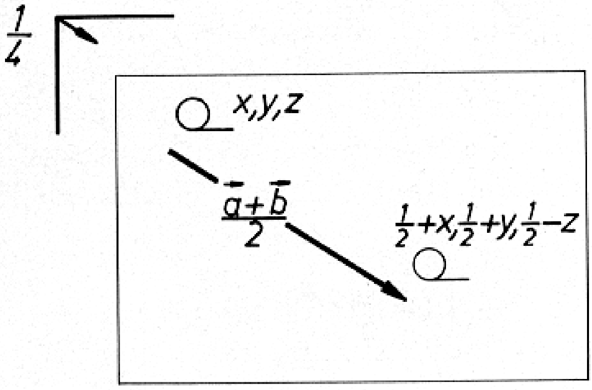


c c-glide at x, $\frac{1}{2}$, z

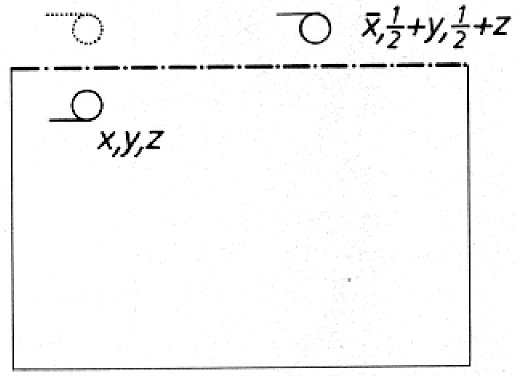
Ott Chap 10

Glide plane

Orthorhombic cell
projected on x,y,o



d n-glide at x, y, $\frac{1}{4}$ with glide component $\frac{1}{2}|\vec{a}+\vec{b}|$



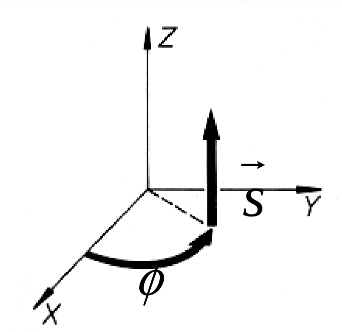
e n-glide at 0, y, z with glide component $\frac{1}{2}|\vec{b}+\vec{c}|$

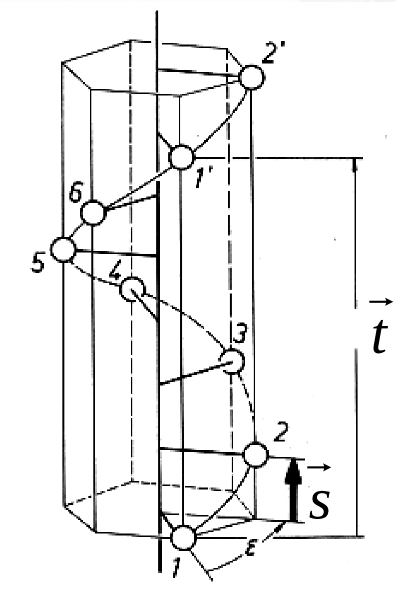
Screw axis

i) rotation $\phi = \frac{2\pi}{X}$ $(X = 1,2,3,4,6)$

ii) translation by a vector $\vec{s}$ parallel to the axis

where $|\vec{s}|$ is called the screw component





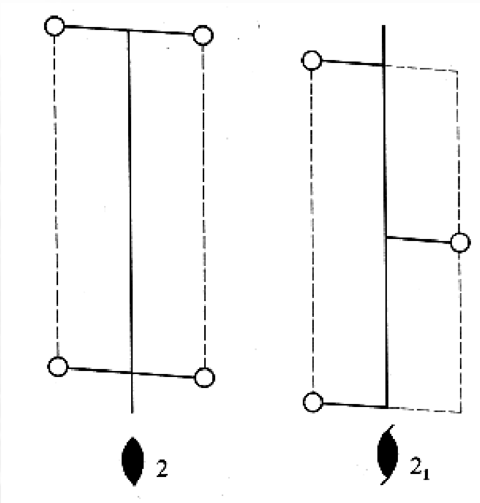
$$|\vec{s}| = \frac{p}{X}|\vec{t}| \quad \text{p=0,1,2...,X-1}$$

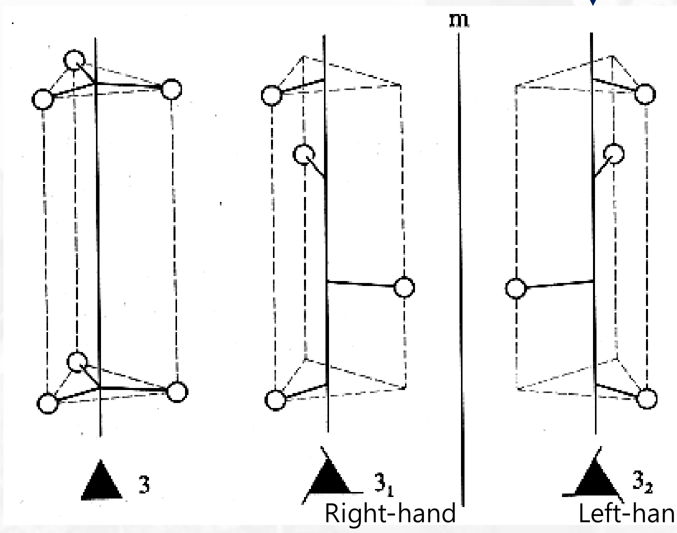
$$X_p = X_0, X_1, \ldots.. X_{X-1}$$

Screw axis

2_1 is a 180º rotation plus ½ cell translation

3_2 is a 120º rotation plus (2/3) cell translation





3_1 is a 120º rotation plus (1/3) cell translation

Screw tetrads

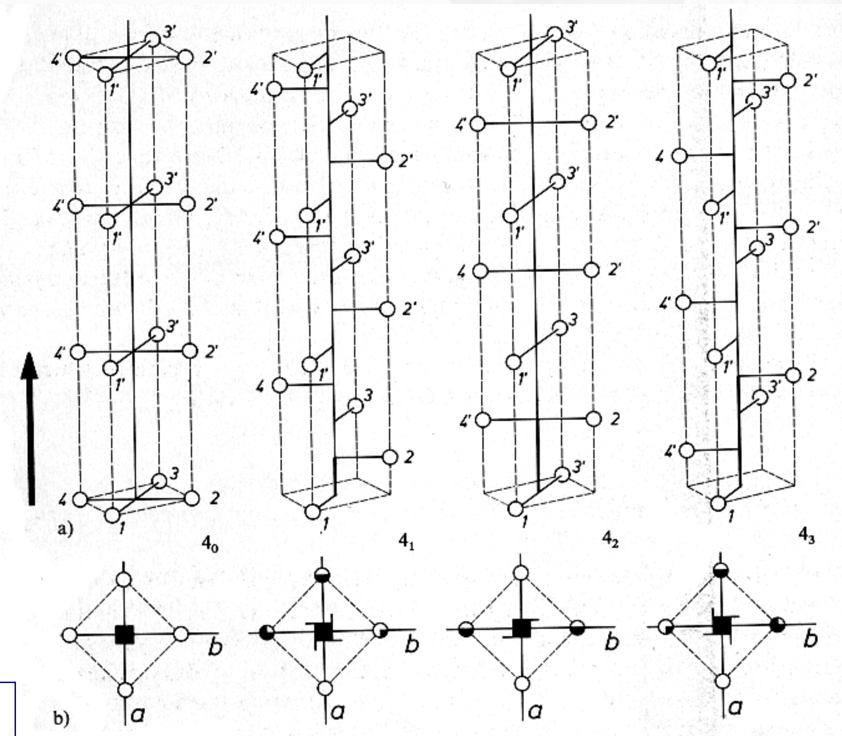
4_0 is 4-fold rotation axis

4_1 is a 90º rotation plus ¼ cell translation (right-handed)

4_2 is a 90º rotation plus ½ cell translation (no handedness)

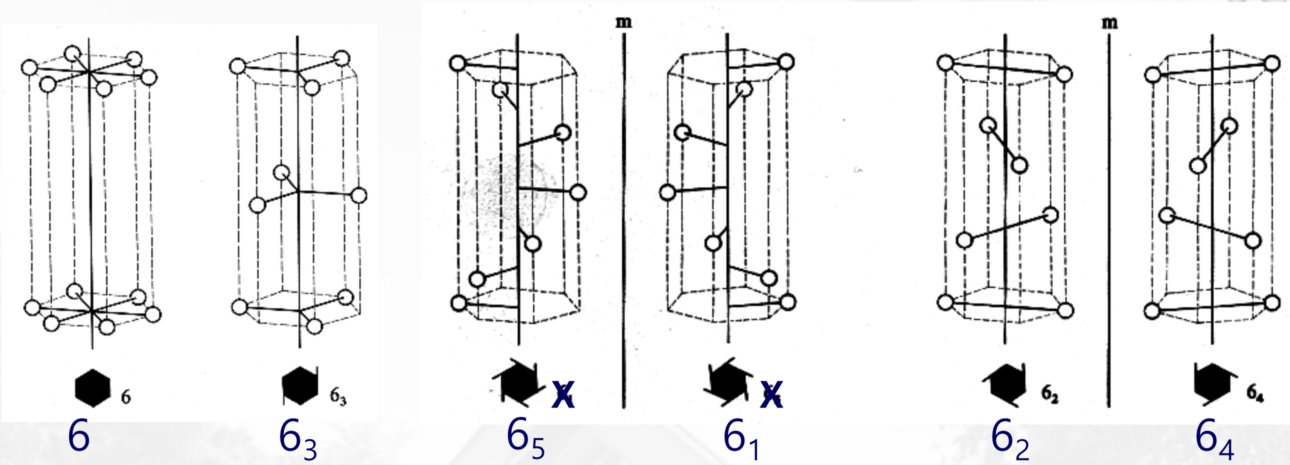
4_3 is a 90º rotation plus ¾ cell translation (right-handed) = a 90º rotation plus ¼ cell translation (left-handed)

Sets of points generated by 4_1 and 4_3 are a pair of enantiomorphs (mirror images of one another)



4_0 4_1 4_2 4_3

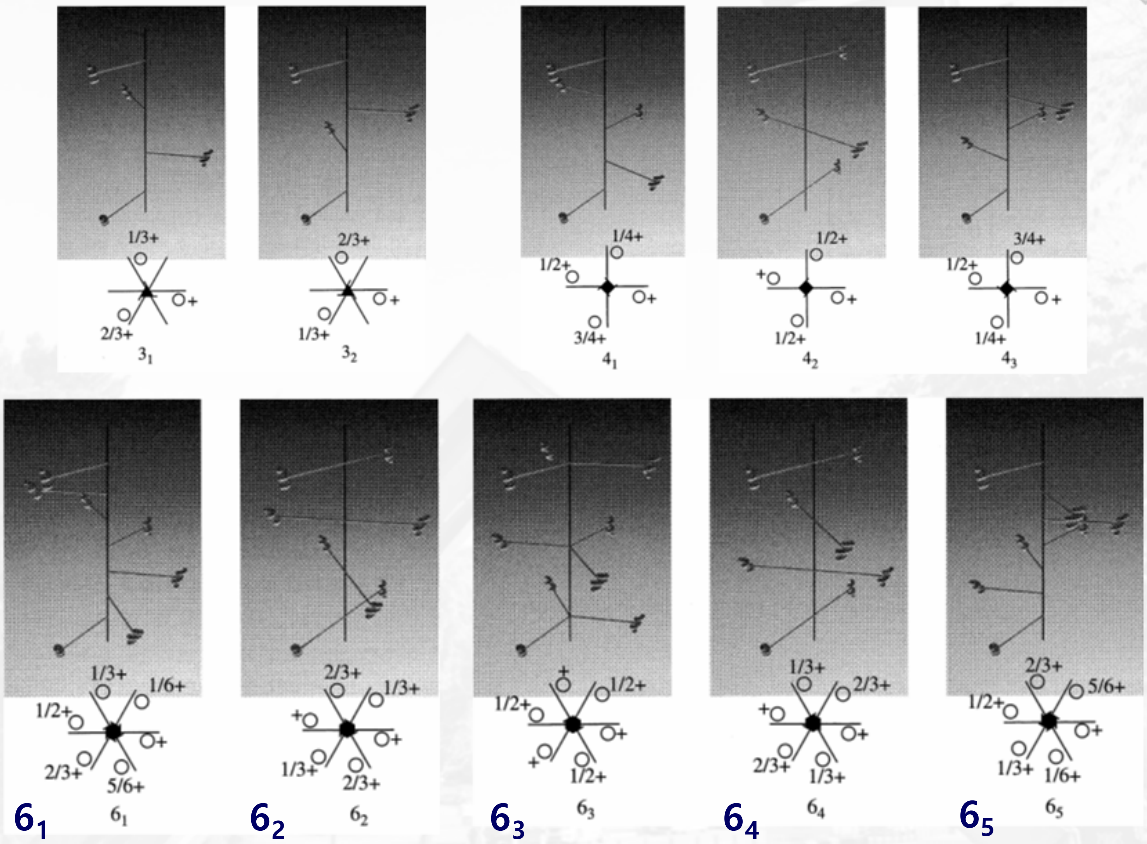
Screw hexads



- **6_1** 60º rotation + 1/6 cell translation (right-handed)
- **6_2** 60º rotation + 1/3 cell translation (right-handed)
- **6_3** 60º rotation + ½ cell translation (no handedness)
- **6_4** 60º rotation + 2/3 cell translation (right-handed) = (1/3 <u>left-handed</u>)
- **6_5** 60º rotation + 5/6 cell translation (right-handed) = (1/6 <u>left-handed</u>)

Screw hexads

page 188, "Structure of Materials", MD Graef & ME McHenry, (2007)

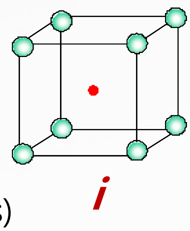


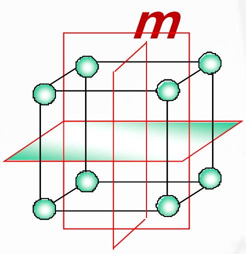
Symbols of symmetry elements

Type of symmetry element	Written symbol	Graphical symbol	
Center of Symmetry	$\bar{1}$	o	
		Perpendicular to paper	In plane of paper
Mirror plane	m		
Glide plane	a b c	glide in plane of paper	arrow shows glide direction
		glide out of plane of paper	
	n		
Rotation	2 3 4 6		
Screw Axis	2_1 3_1 3_2 4_1 4_2 4_3 6_1 6_2 6_3 6_4 6_5		
Inversion Axis	$\bar{3}$ $\bar{4}$ $\bar{6}$		

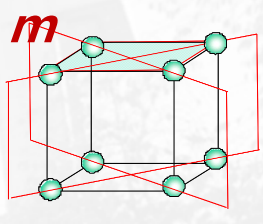
Symmetry elements of a Cube

- center of symmetry
- nine mirror planes
- six diad axes (2-fold rotation axes)
- four triad axes (3-fold rotation axes)
- three tetrad axis (4-fold rotation axes)

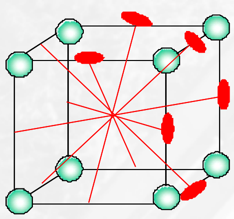




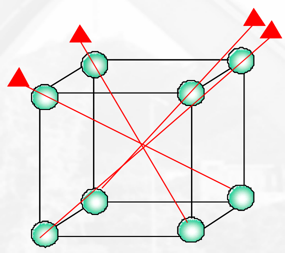
Orthogonal : 3



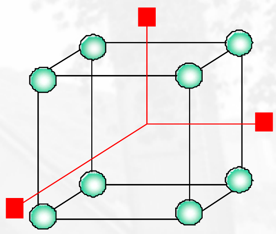
Diagonal : 6



X=2



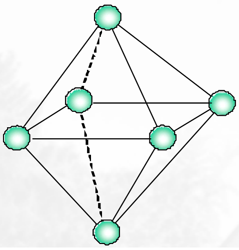
X=3

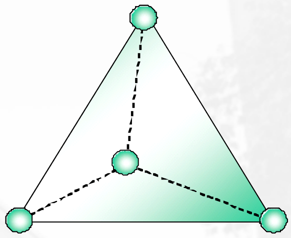


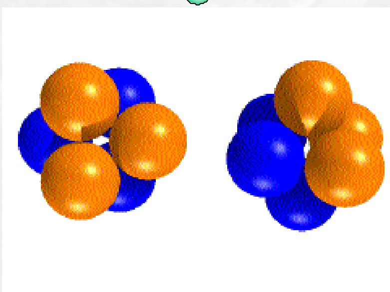
X=4

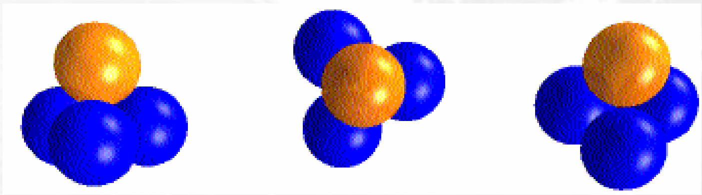
Symmetry elements of Tetrahedron & Octahedron

- Octahedron ; the same symmetry elements as a cube - check this out!
- Tetahedron ; 6 mirror planes, 3 inverse tetrad ($\bar{4}$) axes, 4 triad axes - check this out!









Coordinate Transformation

Algebraic description of symmetry operations

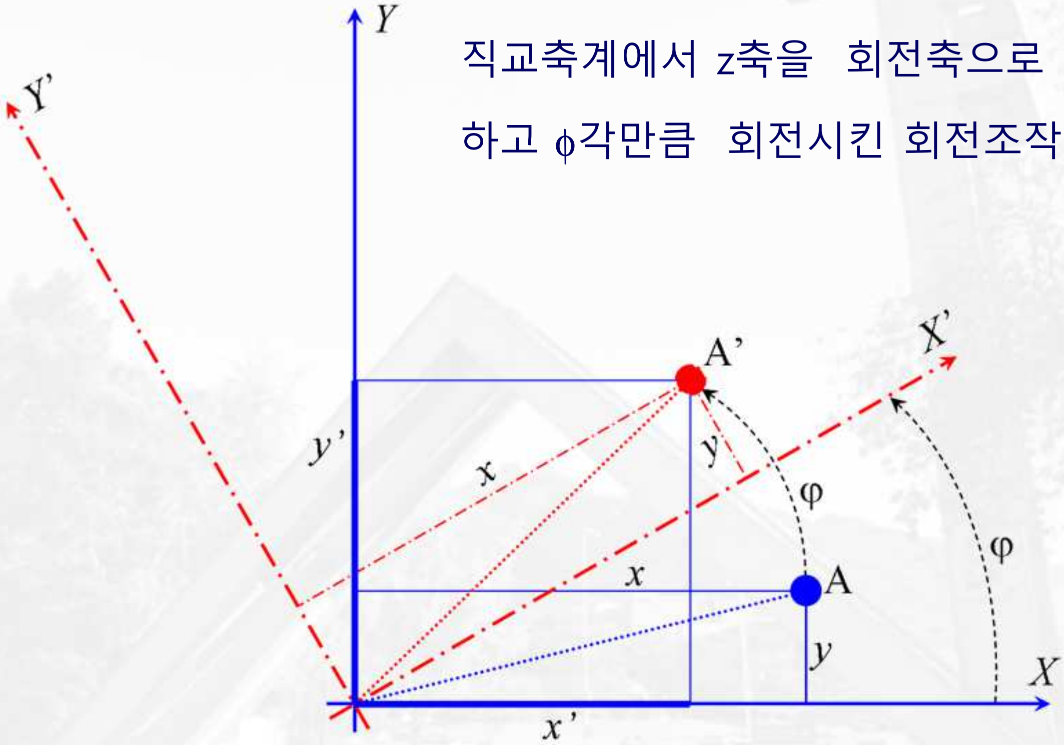
Ott Chap 11

Pecharsky Chap 4.2

Transformation of coordinates of a point

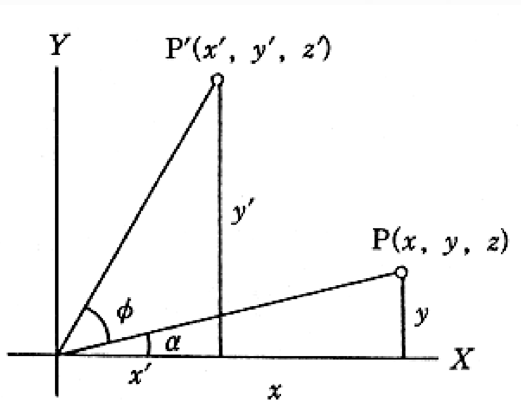
직교축계에서 z축을 회전축으로

하고 φ각만큼 회전시킨 회전조작



Transformation of coordinates of a point - Rotation

- n^i; i times of n-fold rotation operation
  - ✓ $n^1 \bullet n^1 = n^2$, $\quad n^i \bullet n^{n-i} = n^n = 1$
- Matrix representation of rotation in Cartesian coordinate



직교축계에서 z축을 회전축으로 하고 f각만큼 회전시킨 회전조작

$x = r\cos\alpha$, $y = r\sin\alpha$

$x' = r\cos(\alpha + \phi)$

$= r\cos\alpha \cos\phi - r\sin\alpha \sin\phi$

$\underline{x' = x\cos\phi - y\sin\phi}$

$y' = r\sin(\alpha + \phi)$

$= r\sin\alpha \cos\phi + r\cos\alpha \sin\phi$

$\underline{y' = x\sin\phi + y\cos\phi}$

$\underline{z' = z}$

Linear transformation of coordinates on the plane

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Rotation matrix - R

$$R(n_z^1) = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(2_z^1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(3_z^1) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(3_z^2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(4_z^1) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(4_z^2) = R(2_z^1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad R(4_z^3) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$R(4_z^1) \bullet R(4_z^2) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = R(4_z^3)$$

$$R(6_z^1) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

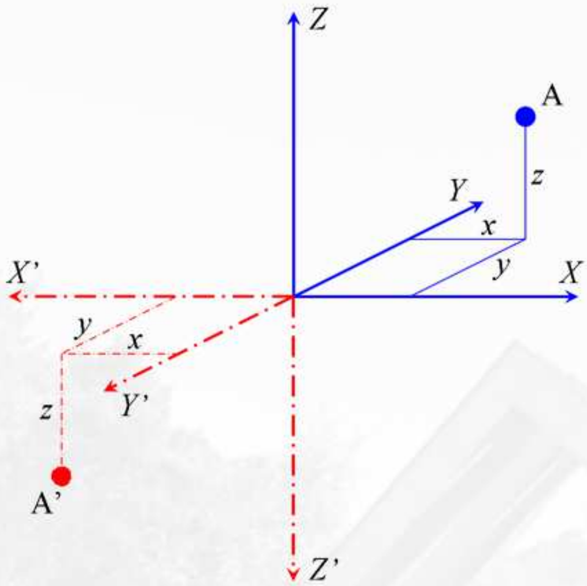
$$R(6_z^2) = R(3_z^1)$$

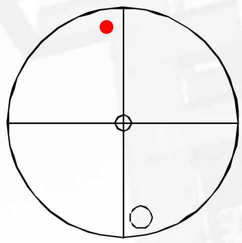
$$R(6_z^3) = R(2_z^1)$$

$$R(6_z^4) = R(3_z^2)$$

$$R(6_z^5) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Inversion





$$\left|R(\bar{1})\right| = -1$$

x' = -x

y' = -y

z' = -z

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad R(\bar{1}) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

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Rotoinversion

rotation

$x' = x\cos\phi - y\sin\phi$

$y' = x\sin\phi + y\cos\phi$

$z' = z$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

inversion

$x' = -x$

$y' = -y$

$z' = -z$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

rotoinversion

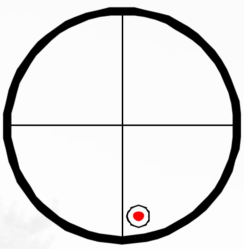
$x' = -x\cos\phi + y\sin\phi$

$y' = -x\sin\phi - y\cos\phi$

$z' = -z$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} -\cos\phi & \sin\phi & 0 \\ -\sin\phi & -\cos\phi & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Reflection

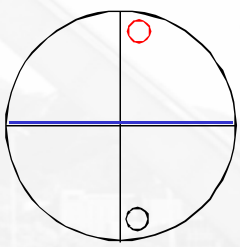


m_{xy} (m_z)

$$x_2 = x_1$$
$$y_2 = y_1$$
$$z_2 = -z_1$$

$$R(m_z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$|R(m_z)| = -1$$



m_{yz} (m_x)

$$x_2 = -x_1$$
$$y_2 = y_1$$
$$z_2 = z_1$$

$$R(m_x) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Transformation of coordinate system

old axis unit vector a, b, c

new axis unit vector a', b', c'

$$a' = p_{11}a + p_{12}b + p_{13}c$$
$$b' = p_{21}a + p_{22}b + p_{23}c$$
$$c' = p_{31}a + p_{32}b + p_{33}c$$

$$\begin{pmatrix} a' \\ b' \\ c' \end{pmatrix} = \begin{pmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix}$$

$$a' = Pa$$

$$a = q_{11}a' + q_{12}b' + q_{13}c'$$
$$b = q_{21}a' + q_{22}b' + q_{23}c'$$
$$c = q_{31}a' + q_{32}b' + q_{33}c'$$

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{pmatrix} \begin{pmatrix} a' \\ b' \\ c' \end{pmatrix}$$

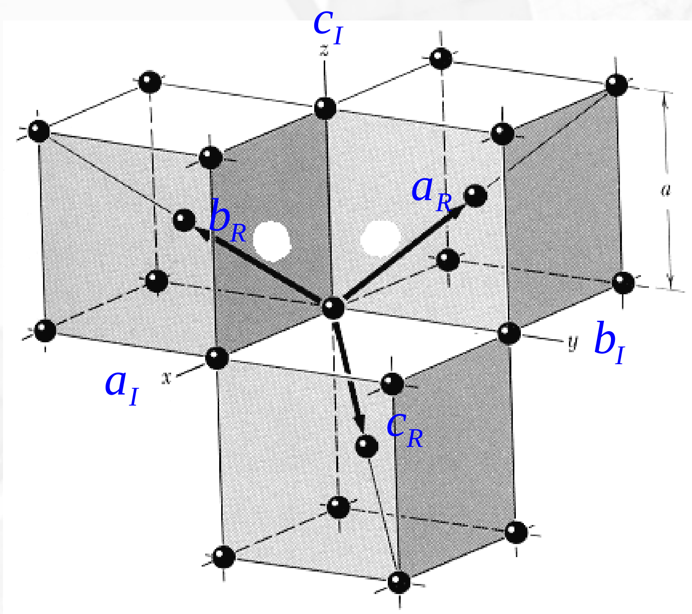
$$a = Qa' \qquad PQ = I$$

Transformation of coordinate system

bcc to rhombohedral

$$a_R = -\frac{1}{2}a_I + \frac{1}{2}b_I + \frac{1}{2}c_I$$
$$b_R = \frac{1}{2}a_I - \frac{1}{2}b_I + \frac{1}{2}c_I$$
$$c_R = \frac{1}{2}a_I + \frac{1}{2}b_I - \frac{1}{2}c_I$$

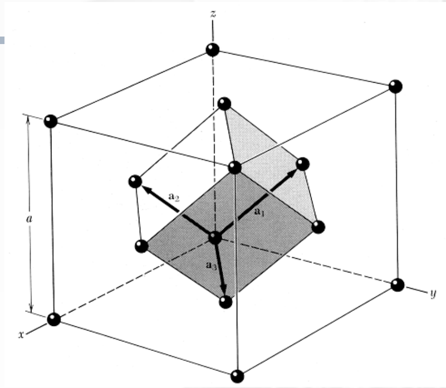
$$a_I = 0a_R + 1b_R + 1c_R$$
$$b_I = 1a_R + 0b_R + 1c_R$$
$$c_I = 1a_R + 1b_R + 0c_R$$



$$P = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix} \qquad Q = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}$$

Transformation of coordinate system

fcc to rhombohedral



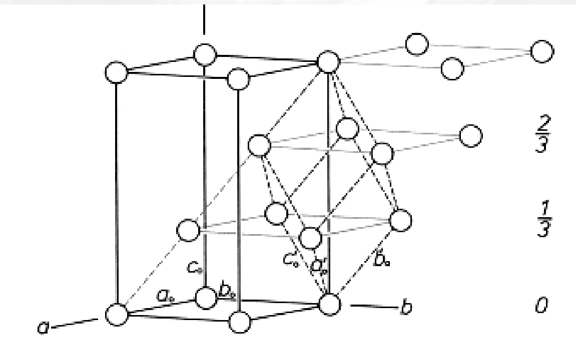
$a_o = b_o \neq c_o$

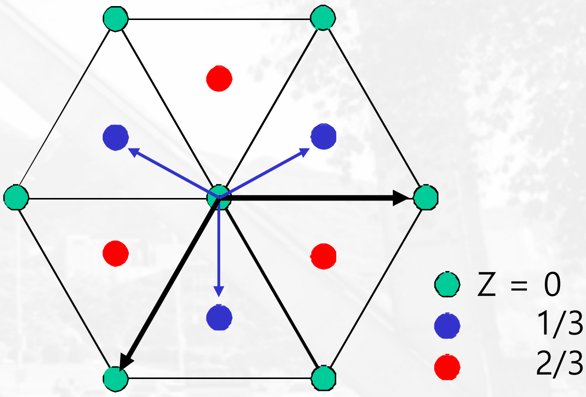
$\alpha = \beta = 90^o \quad \gamma = 120^o$

$a_o' = b_o' = c_o'$

$\alpha = \beta = \gamma$

trigonal R - rhombohedral P





Ott page 88, page 267

todos

Read

- ✓ Ott Chapter 6; 10.1
- ✓ Sherwood & Cooper Chapter 3.6
- ✓ Hammond Chapter 2.1 ~ 2.3; 12.5.1; 12.5.2
- ✓ Krawitz Chapter 1.1 ~ 1.3

Use

- ✓ http://materials.cmu.edu/degraef/pg/pg_gif.html
- ✓ http://neon.mems.cmu.edu/degraef/pg/pg.html#AGM

➢ Symmetry HW (due in 1 week)

- ✓ Ott chapter 6 --- 1, 3, 4, 5, 6, 9
- ✓ Ott chapter 7 --- 1, 2, 3, 4, 5, 9