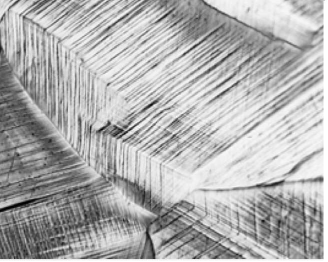
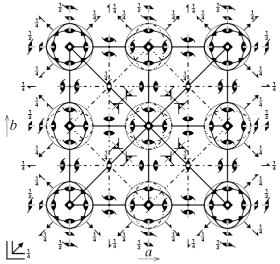
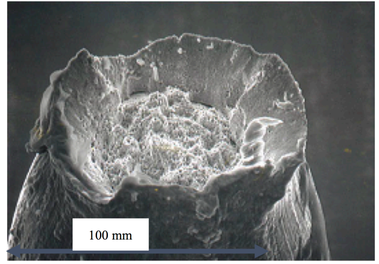
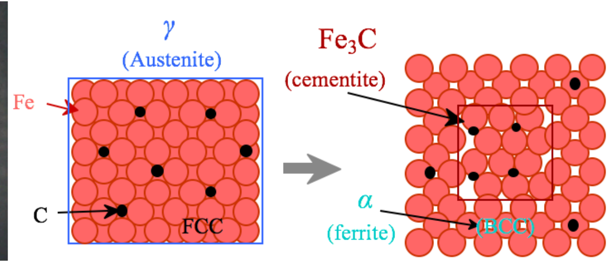








MEAM/MSE 507
Fundamentals of Materials

Prof. Jordan R. Raney

Week 4, Lecture 3: Crystallographic notation (part 1)

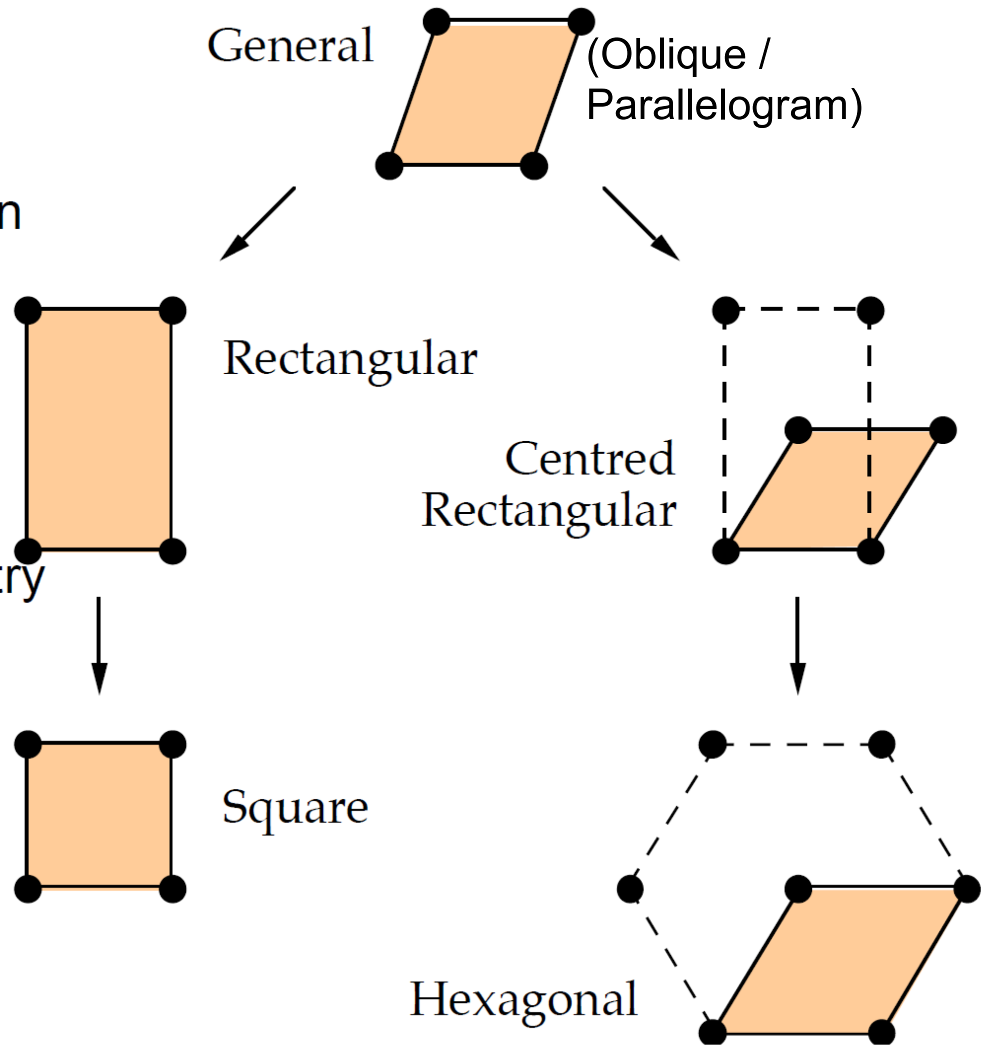
Asynchronous

Bravais lattices in 2D

- Bravais lattice is an infinite array of discrete points generated by

$$\boldsymbol{R}_{\mathrm{lmn}} = \mathrm{l}\boldsymbol{a} + \mathrm{m}\boldsymbol{b} + \mathrm{n}\boldsymbol{c}$$

- Infinite number of space lattices can be formed by choosing $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ in 3d or $\boldsymbol{a}$, $\boldsymbol{b}$ in 2d
- From any R_{lmn} the lattice looks exactly the same
- Most lattices only have the symmetry n=1 or 2, but we can choose $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ to get other symmetries
- These symmetries imply restriction on $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$
- Each set of restrictions → distinct lattice; a Bravais lattice is characterized by its symmetry operations



2d: 4 restrictions→ 5 lattices

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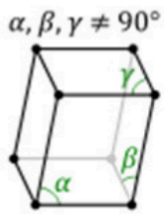
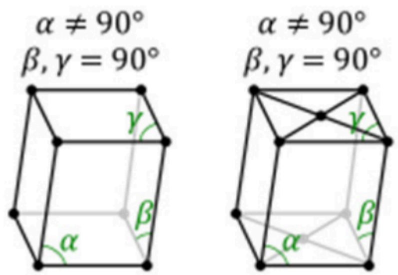
Bravais lattices in 3D

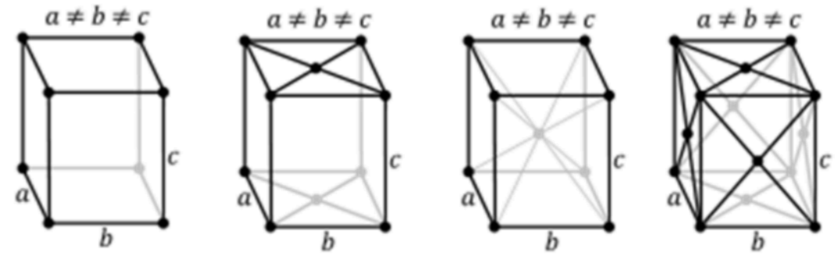
Triclinic



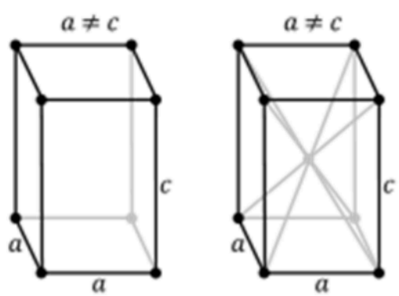
Monoclinic



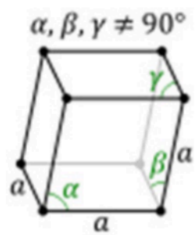
Orthorhombic



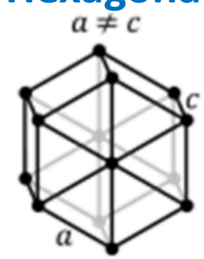
Tetragonal



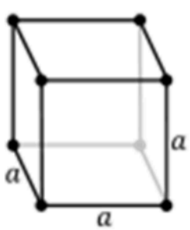
Trigonal/rhombohedral



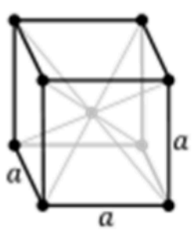
Hexagonal



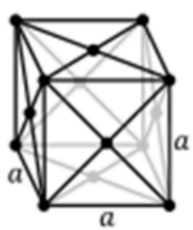
Cubic



Simple Cubic



Body Centered Cubic



Face Centered Cubic

- **14 Bravais lattices in 3D**
- **7 crystal systems**

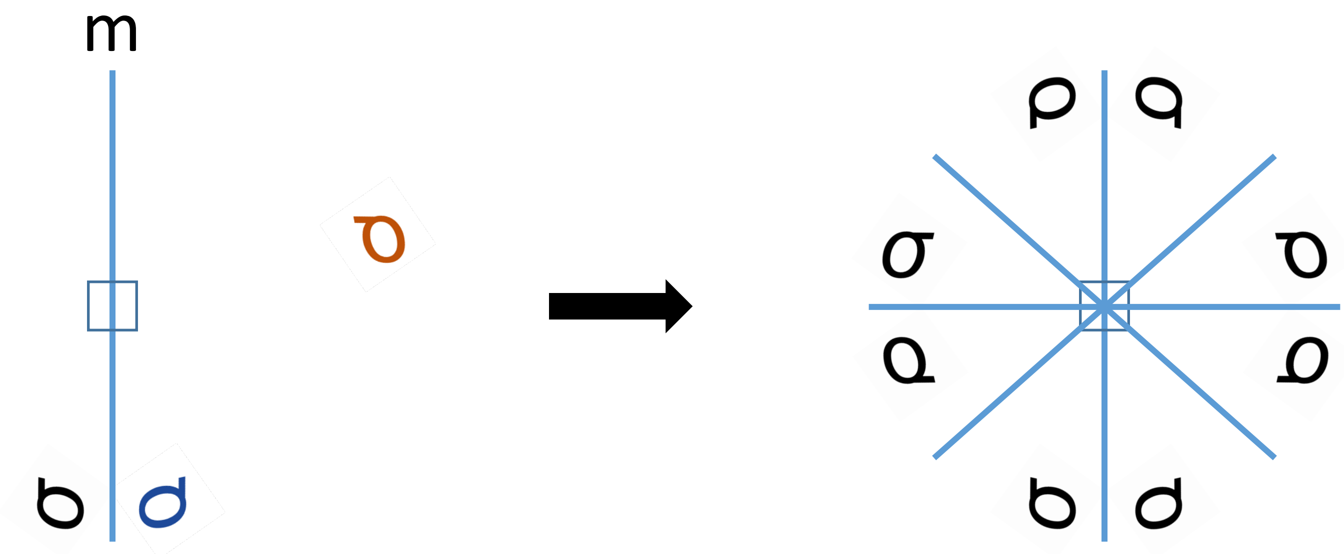
Point group notation

- Point groups describe symmetries with respect to specific points
- These do not involve translation operations

X	Rotation by $2\pi/X$
$\bar{X}$	Inversion axis – invert then rotation by $2\pi/X$
$X2$	Rotation by $2\pi/X$ + subsidiary 2-fold rotation axis perpendicular to the X-axis
$\bar{X}2$	Rotary inversion by $2\pi/X$ + subsidiary 2-fold rotation axis perpendicular to the $\bar{X}$-axis
Xm	Rotation by $2\pi/X$ + a mirror containing the X-fold rotation axis
$\bar{X}m$	Rotary inversion by $2\pi/X$ + a mirror containing the X-fold rotation axis
X/m	Rotation by $2\pi/X$ + a mirror perpendicular to the X-fold rotation axis
$\bar{X}/m$	Rotary inversion by $2\pi/X$ + a mirror perpendicular to the X-fold rotation axis
X/mm	Rotation by $2\pi/X$ + a mirror containing and a mirror perpendicular to the X-fold rotation axis
mm	2 mutually orthogonal mirror planes
$\bar{X}2m$	A mirror plane that contains $\bar{X}$ and 2-fold rotation

- Why the word "group"?

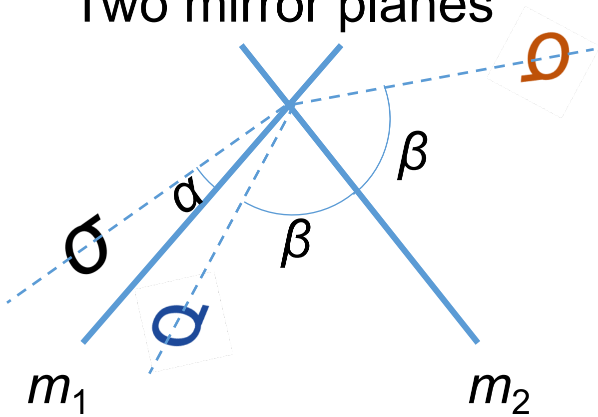
Point group example (2D)



- Notation: running list of independent symmetry elements
- **4mm**
- (Not 4mmmmmmmm or 4mmmm – only 2 kinds of mirrors)

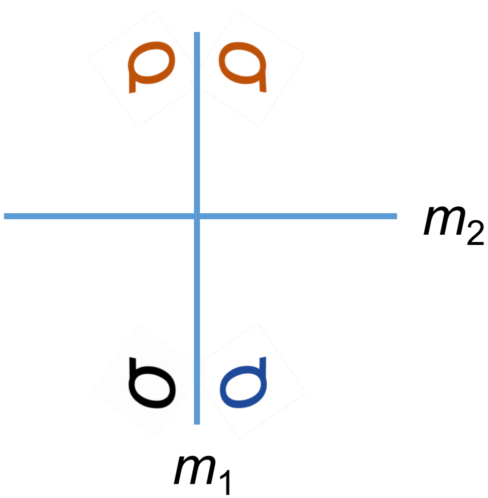
Combinations of operators

Two mirror planes



- Notice chirality L -> R -> L
- **Two sequential reflections** via mirrors m_1 and m_2, separated by an angle $\alpha+\beta$
- **Equivalent to a single rotation** $A_{2(\alpha+\beta)}$
- These are members of a Group

Example (Group 2mm)



E.g., $m_2 \cdot m_1 = A_\pi$

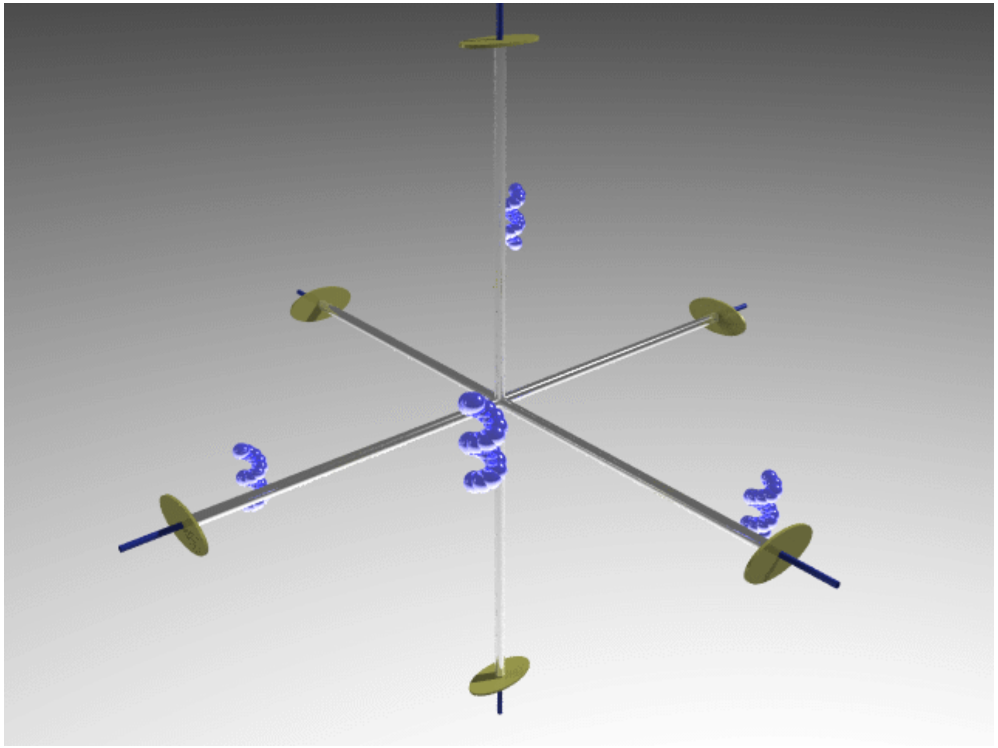
	1	$\boldsymbol{m_1}$	$\boldsymbol{m_2}$	$\boldsymbol{A_\pi}$
1	1	m_1	m_2	A_π
$\boldsymbol{m_1}$	m_1	1	A_π	m_2
$\boldsymbol{m_2}$	m_2	A_π	1	m_1
$\boldsymbol{A_\pi}$	A_π	m_2	m_1	1

- Group of rank 4
- Notice also that there are 4 motifs….
- Tells you how to map any one of the motifs into all others (and itself)

Point groups in 3D

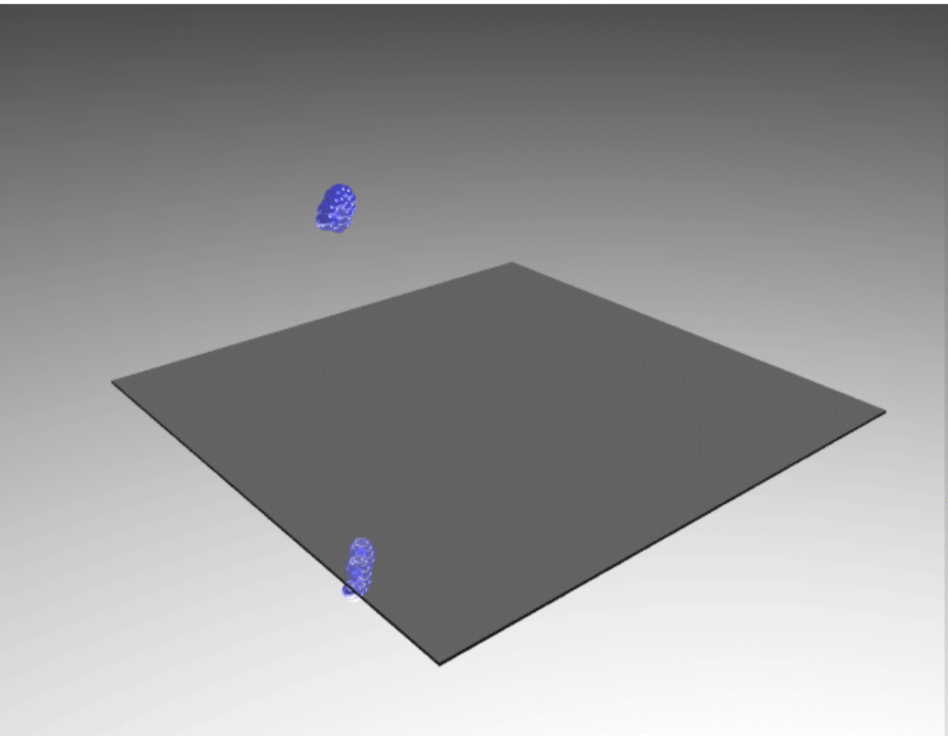
Rotation limitations are the same as in 2D (sometimes called "cyclic" symmetry and designated C_1, C_2, C_3, C_4, C_6)

E.g., Dihedral point group 222 (2-fold symmetries along *x*, *y*, and *z* directions, giving group members $\{1, 2_z, 2_y, 2_x\}$)

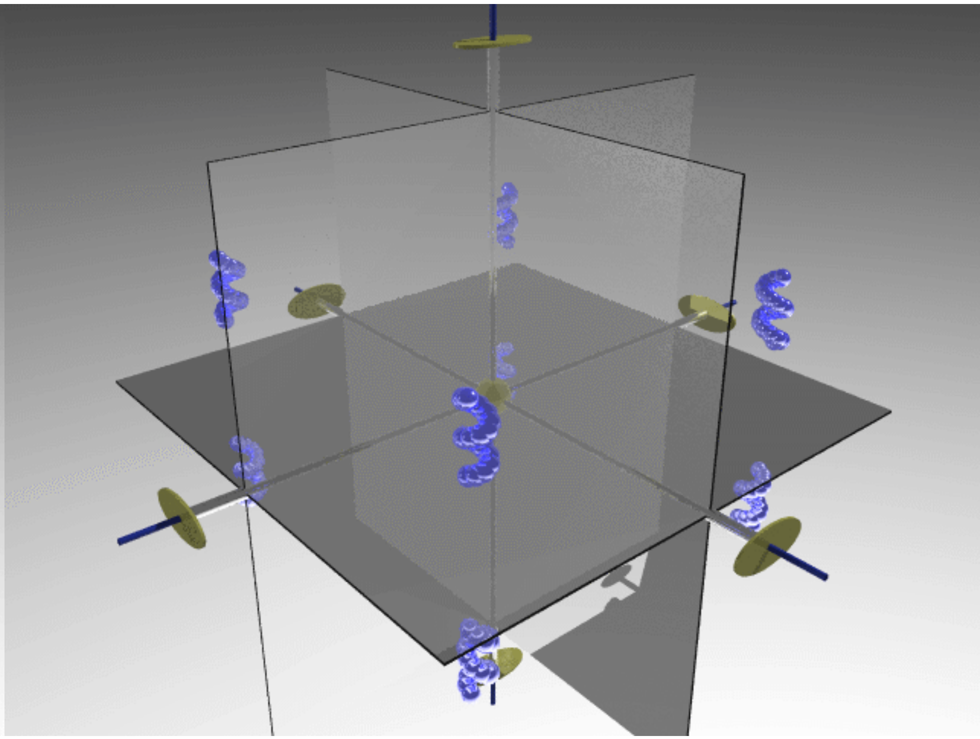


Point group notation

m



mmm

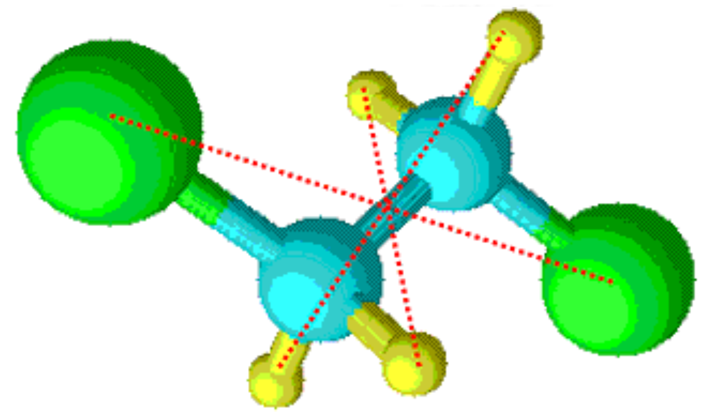


See additional animations at:
http://www.xtal.iqfr.csic.es/Cristalografia/parte_03-en.html

Inversion (an additional operation in 3D)

Inversion

- Inversion (center of symmetry)
- Reflection of every point through the center, $\bar{1}$



$$(x,y,z) \rightarrow (-x, -y, -z)$$

Rotary inversion

- Rotation by n-fold axis + inversion, $\bar{n}$
- Note, this does not imply that there is an n-fold rotation axis
- Also called improper rotation or rotary reflection depending on plane of inversion

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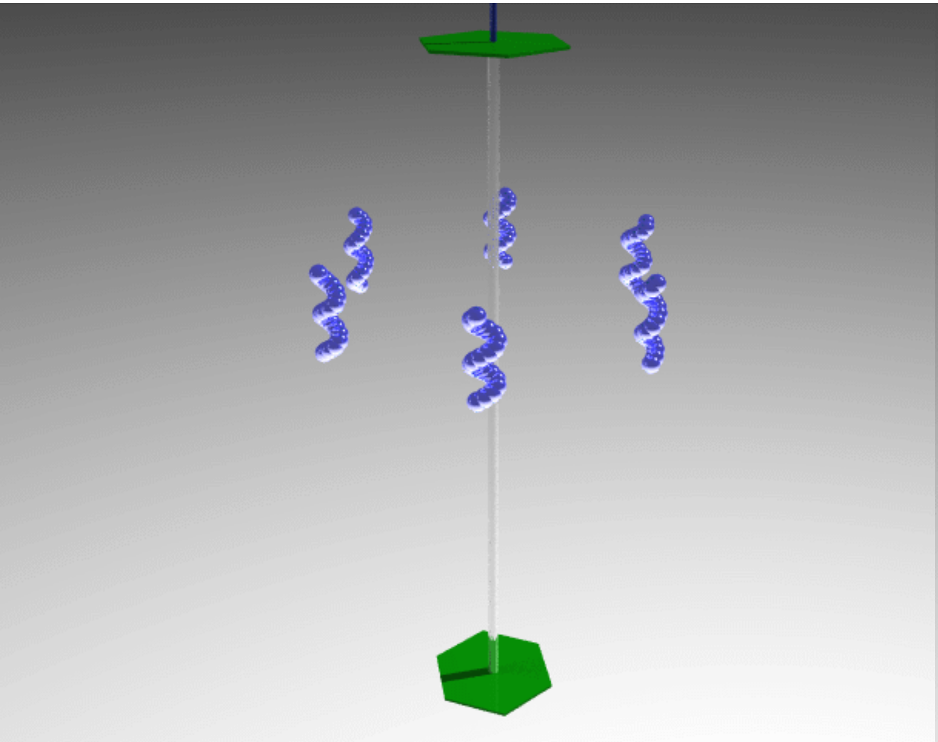
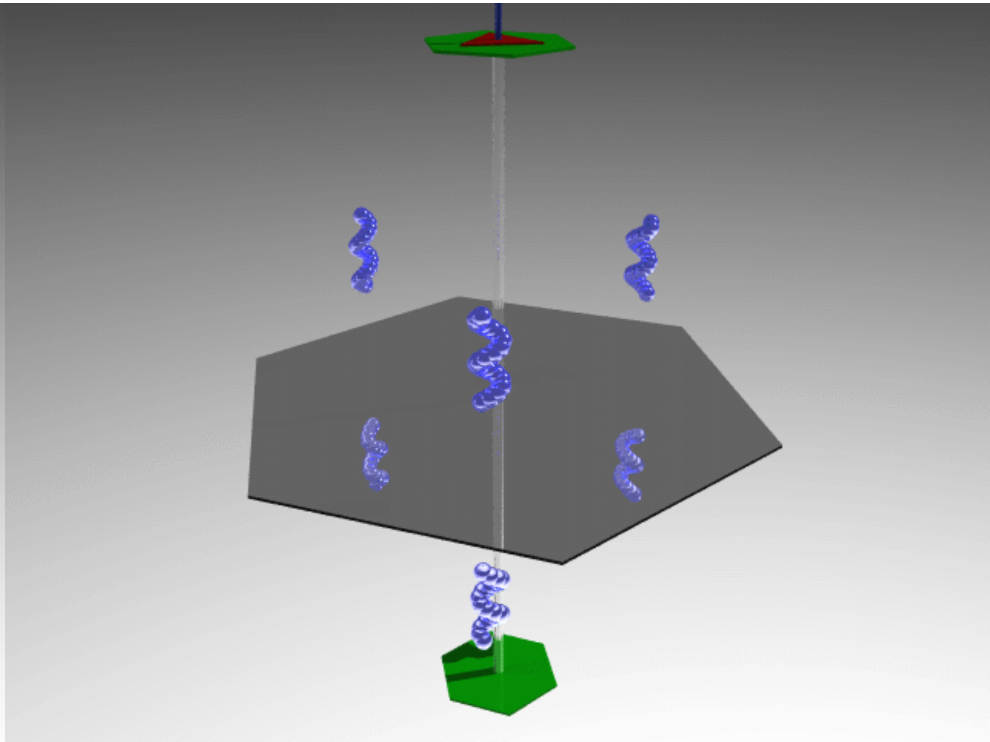
Point group notation

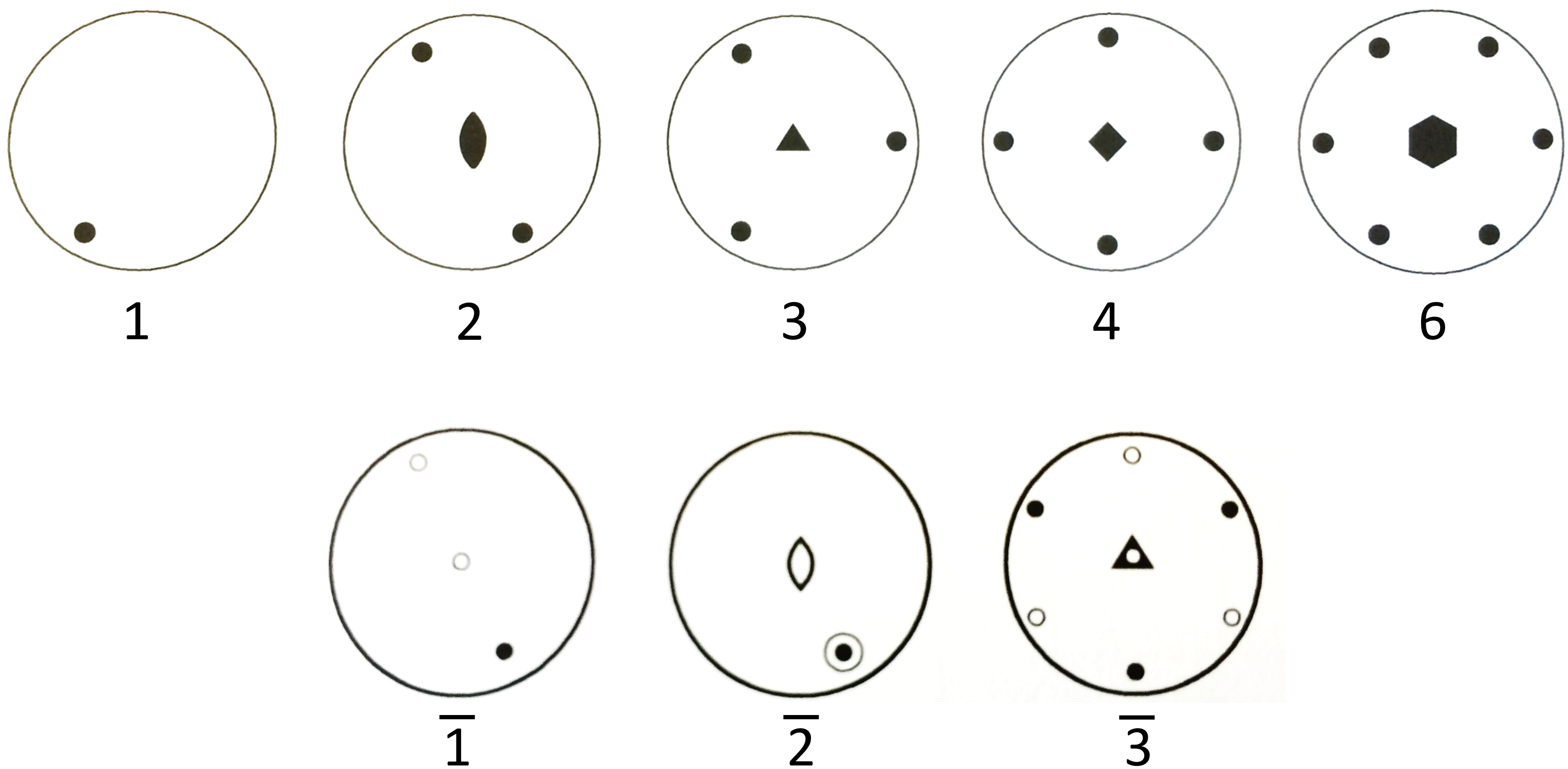
6



$\bar{6}$



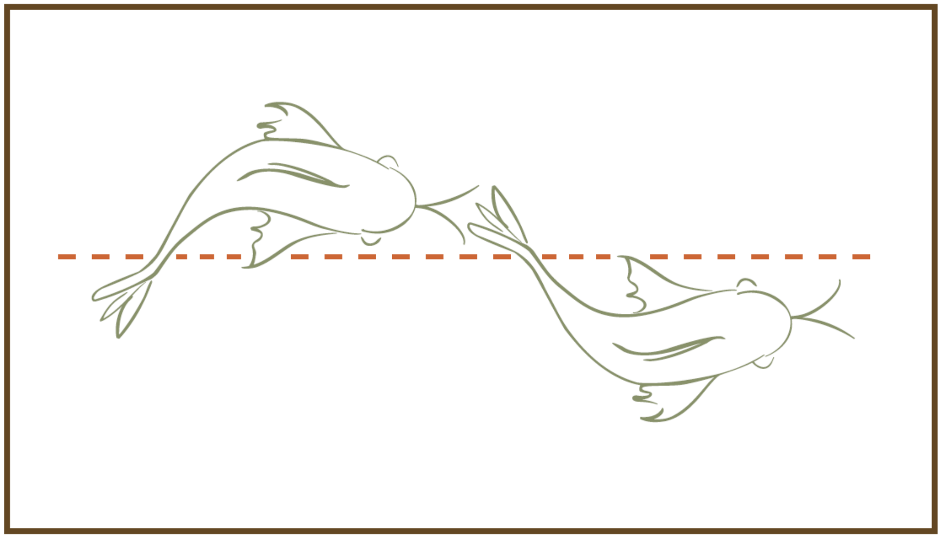
Stereographic projections

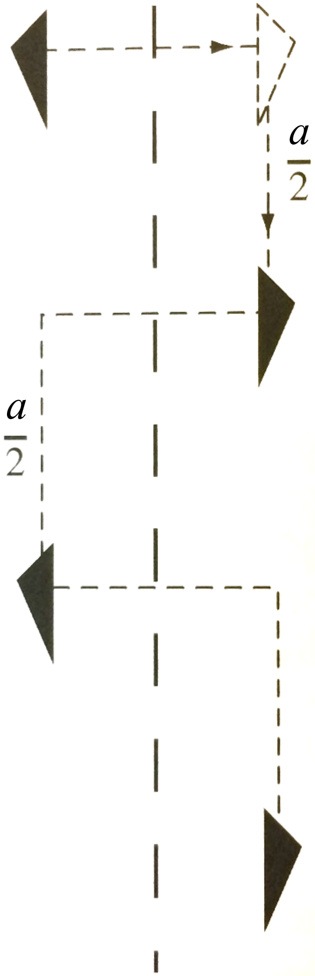


- Represents top down view of 3D sphere projected onto 2D plane (our view is from the “North pole”)
- Black dot is projected in the northern hemisphere
- Circle is underneath, on the southern hemisphere

Glide (2D or 3D)

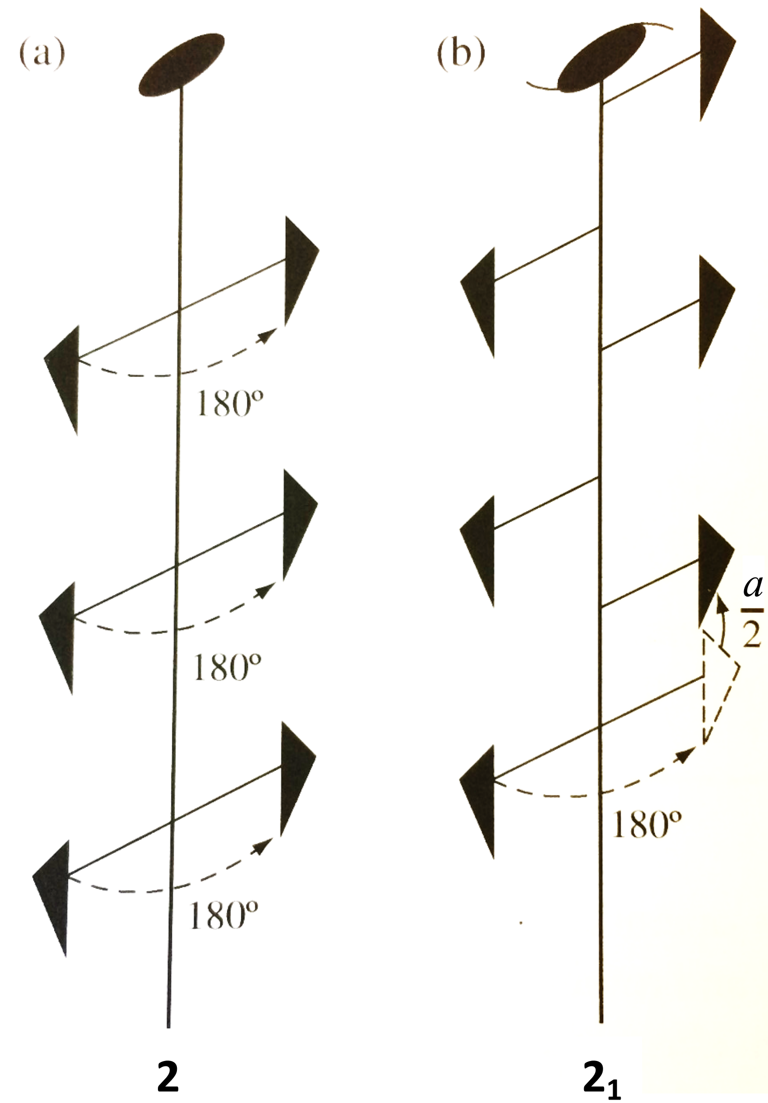
- Glide = Reflection + Translation
- Represented by a dashed line
- In a crystal with lattice parameter *a*, the translation is *a*/2
- In 2D, a glide operation is associated with a glide line
- In 3D, a glide operation is associated with a glide plane





Screw (3D only)

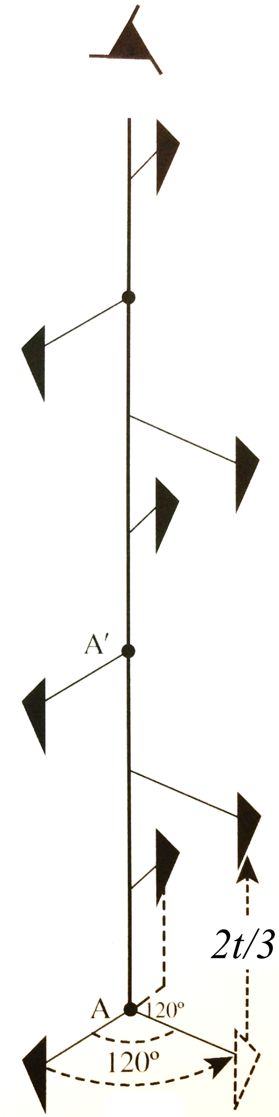
- Screw = Rotation + Translation
- In a crystal with lattice parameter *a*, the screw operation n_m is an *n*-fold rotation followed by a translation of $a(m/n)$
- E.g., 6_3 is a rotation of $2\pi/6$ and a translation of $(3/6)a$ or $a/2$.



Screw

Name	Symbol	Graphical symbol	Right-handed screw translation along the axis in units of the lattice parameter
Screw diad	2_1		$\frac{1}{2}$
Screw triads	3_1		$\frac{1}{3}$
	3_2		$\frac{2}{3}$
Screw tetrads	4_1		$\frac{1}{4}$
	4_2		$\frac{2}{4} = \frac{1}{2}$
	4_3		$\frac{3}{4}$
Screw hexads	6_1		$\frac{1}{6}$
	6_2		$\frac{2}{6} = \frac{1}{3}$
	6_3		$\frac{3}{6} = \frac{1}{2}$
	6_4		$\frac{4}{6} = \frac{2}{3}$
	6_5		$\frac{5}{6}$

Crystallography and Crystal Defects, Kelly & Knowles



$\mathbf{3_2}$