ME 5374-ST

Machine Learning for Materials Science and Discovery

Fall 2025

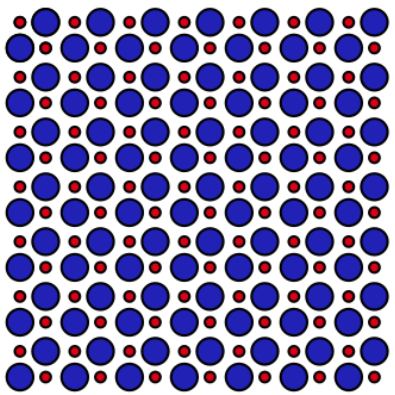
Asst. Prof. Peter Schindler

Lecture 7 – Crystallography Crash Course and Pymatgen

- Lattices and Unit Cells
- 2D and 3D Bravais Lattices
- Symmetry in Crystals
- Crystallographic Point Groups and Space Groups
- Closed Packed and Other Common Crystal Structures
- Fractional/Cartesian Coordinates and the Metric Tensor

Order in Materials

Crystalline
3D long range order
repeating *unit cell*

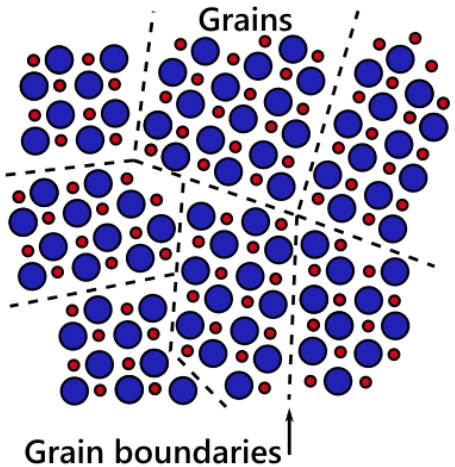


Si wafer

Diamond

Minerals

Polycrystalline
Medium range order
Grains separated by GB



random / textured

Gate electrode in transistor
Aluminum contacts
Metals

Soft matter

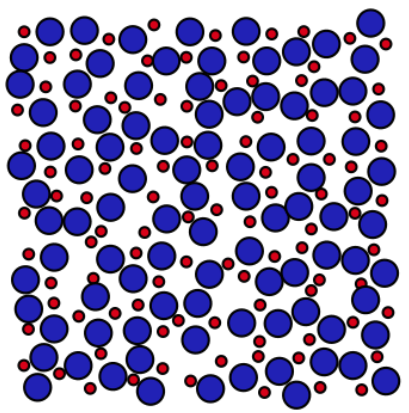
Liquid Crystal

Semi-Crystalline

Quasi-Crystal

Nanocrystals

Amorphous
No order
(only short range)



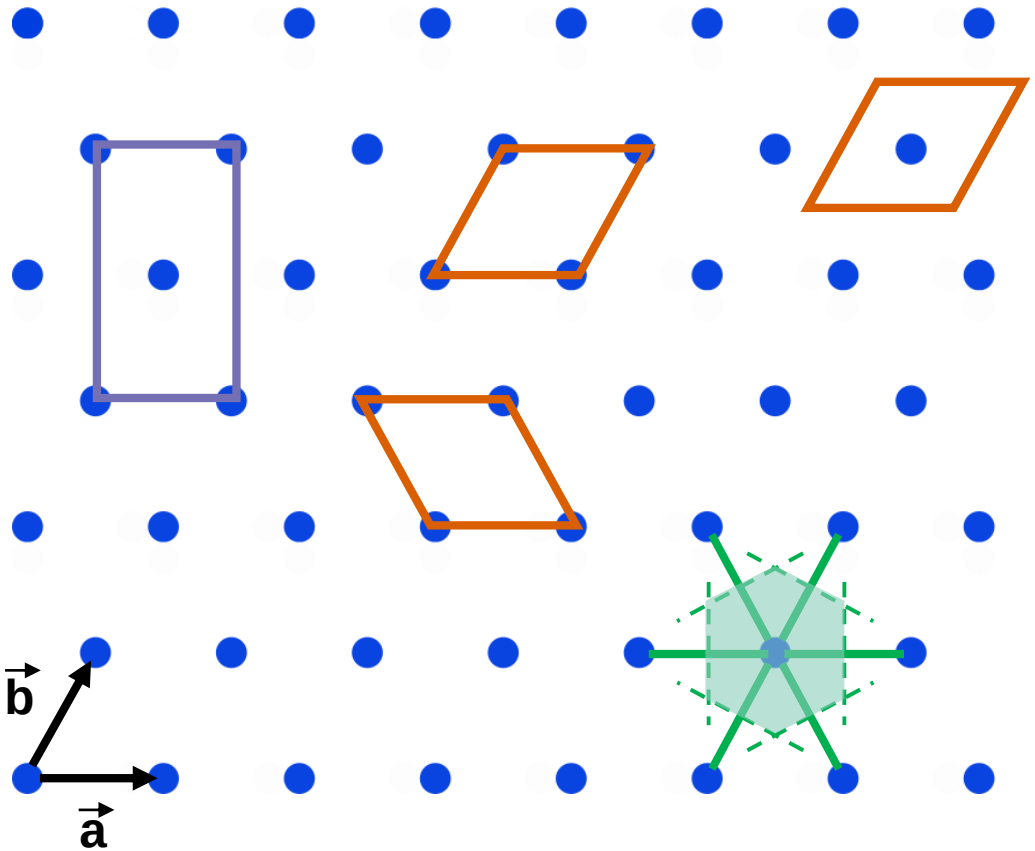
Gate oxide in transistor

Glass

Ceramics

Lattice and Unit Cells

Lattice = infinite arrangement of points in space; each point has *identical surroundings*



Unit cell

Volume that if repeated by lattice vectors covers the entire lattice (no gaps/holes)

-not unique

Primitive unit cell

Unit cell with only one lattice point (= smallest unit cell)

[not always used for visualization]

-not unique

Wigner-Seitz cell

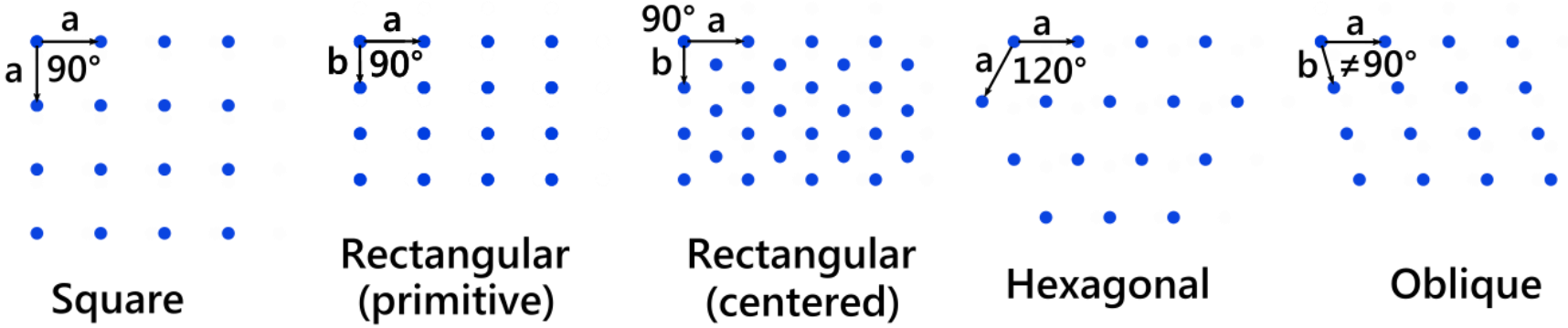
Volume that's closer to a specific lattice point than to any other;

is also a primitive unit cell

-unique

Unique Lattices in 2D and 3D

In **2D → 5** unique unit cell shapes called **Bravais** lattices:



In **3D → 7 lattice systems** and **4 centering types** → **14 Bravais lattices**

Triclinic, Monoclinic,
Orthorhombic, Tetragonal,
Hexagonal, Rhombohedral
and Cubic

P Primitive
I Body centered
F Face centered
C Base centered

Crystal = Lattice + Motif (also called 'basis')

7 lattice systems (define valid periodic tilings) → 32 point groups

14 Bravais lattices (define valid translations) → 230 space groups

14 Bravais Lattices

Lattices in 3D:

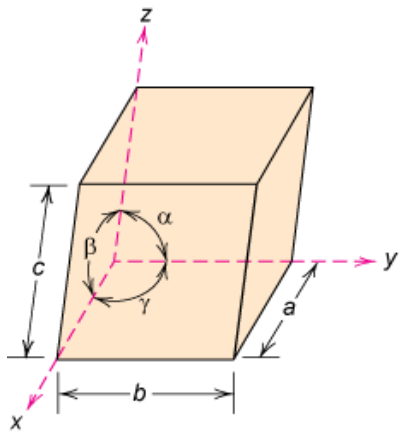
Defined by

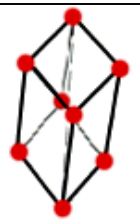
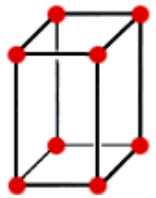
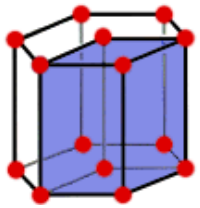
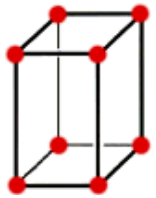
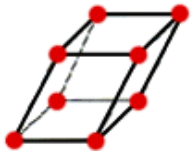
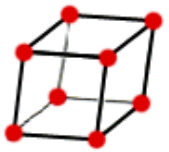
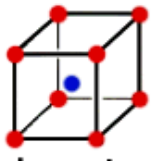
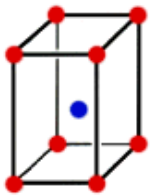
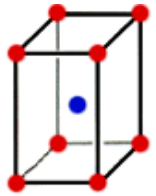
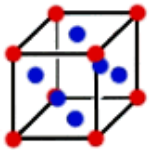
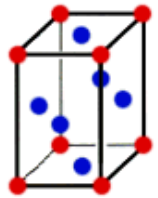
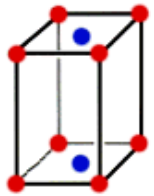
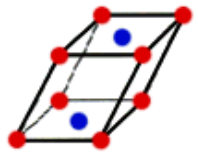
unit cell vectors:

$$\{\vec{e}_i\} = \{\vec{a}, \vec{b}, \vec{c}\}$$

or lattice parameters

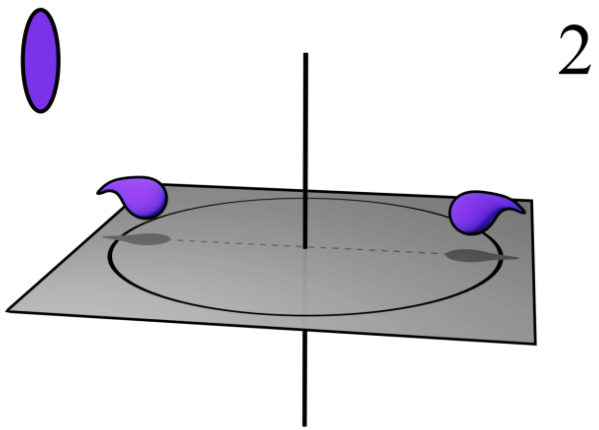
$$\{a, b, c, \alpha, \beta, \gamma\}$$

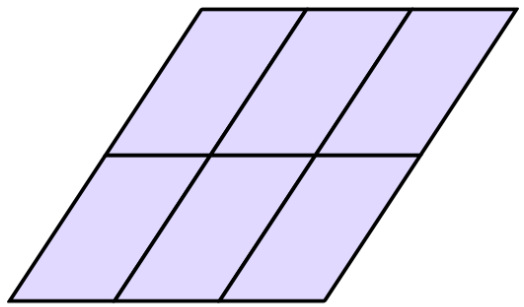


	Cubic	Rhombohedral	Tetragonal	Hexagonal	Orthorhombic	Monoclinic	Triclinic
P Primitive							
I Body centered							
F Face centered							
C Base centered							

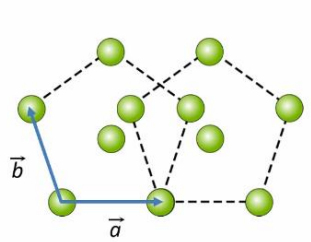
Symmetry in Crystals

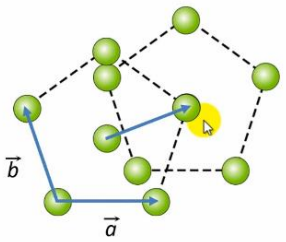
Rotational symmetry



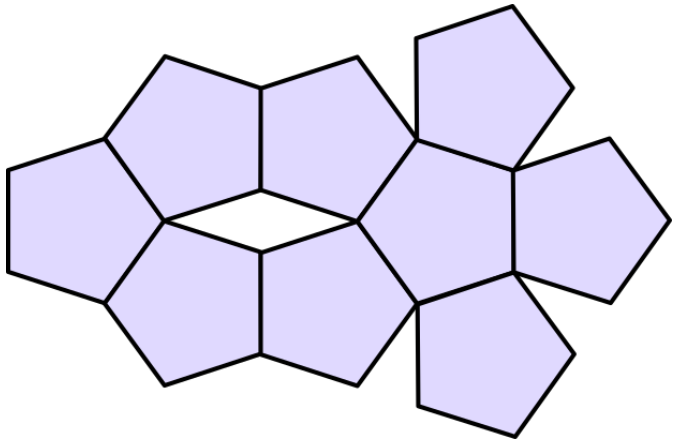


2-fold (180°)



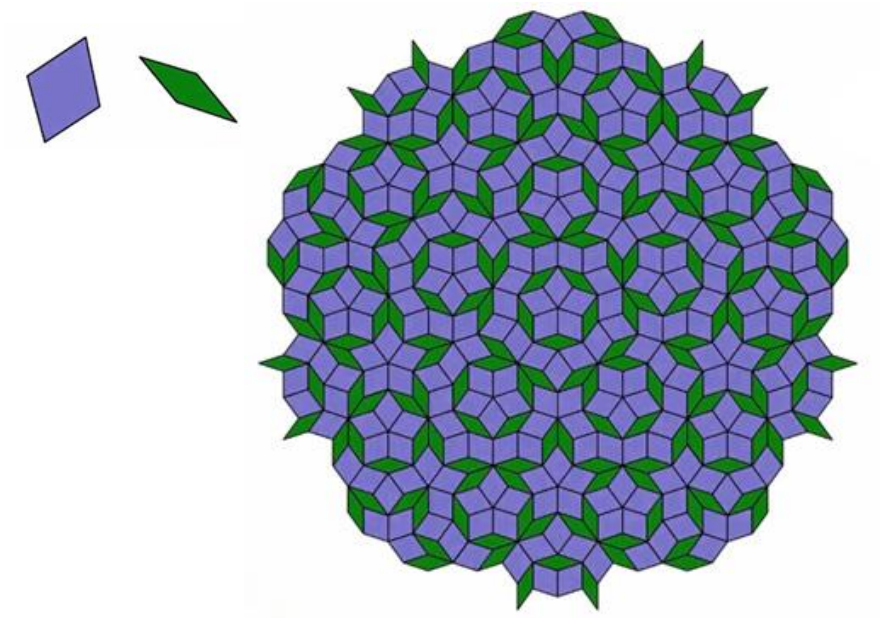


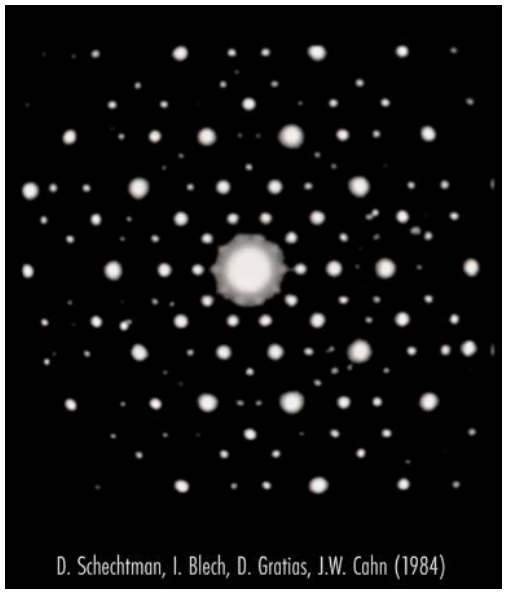
Pentagons *do not* tile the plane without **gaps**



Symmetry in Crystals

https://www.youtube.com/watch?v=48sCx-wBs34
https://csfulop.github.io/PenroseMoire/?x=212?y=0?r=0



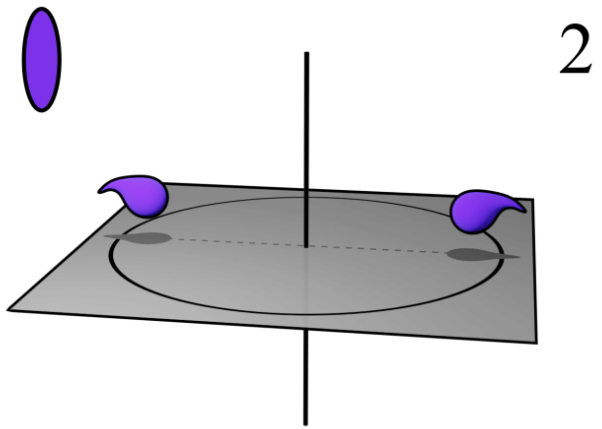


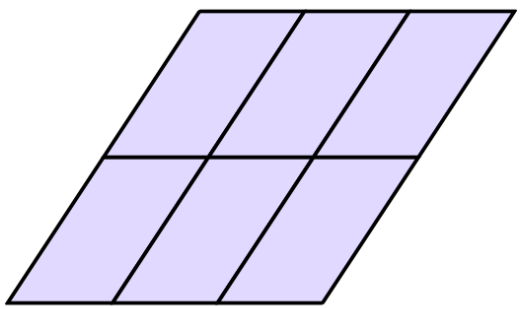
Al_6Mn, D. Schechtman
Chemistry Nobel prize 2011

L. Pauling: "*There are no quasicrystals, only quasi-scientist*"

Symmetry in Crystals

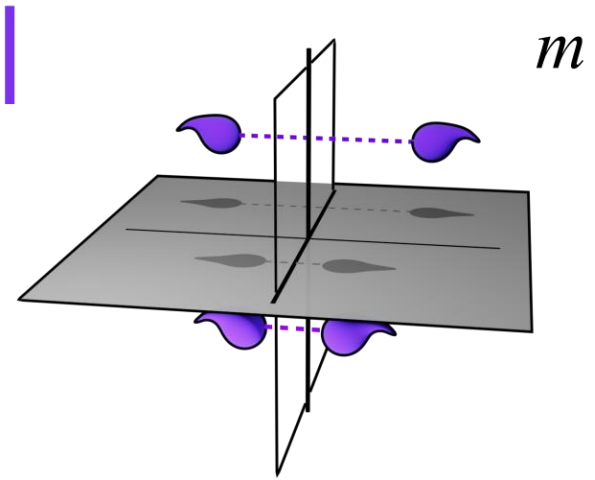
Rotational symmetry



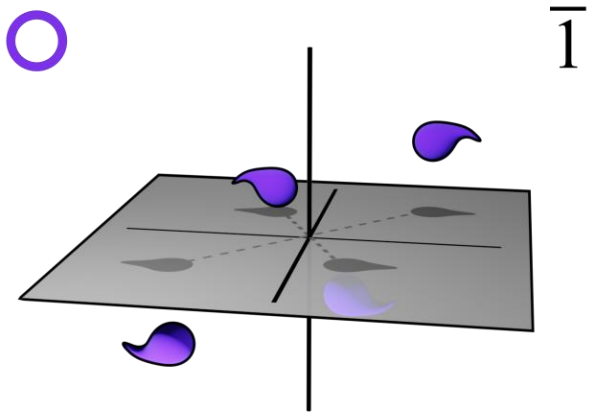


2-fold (180°)

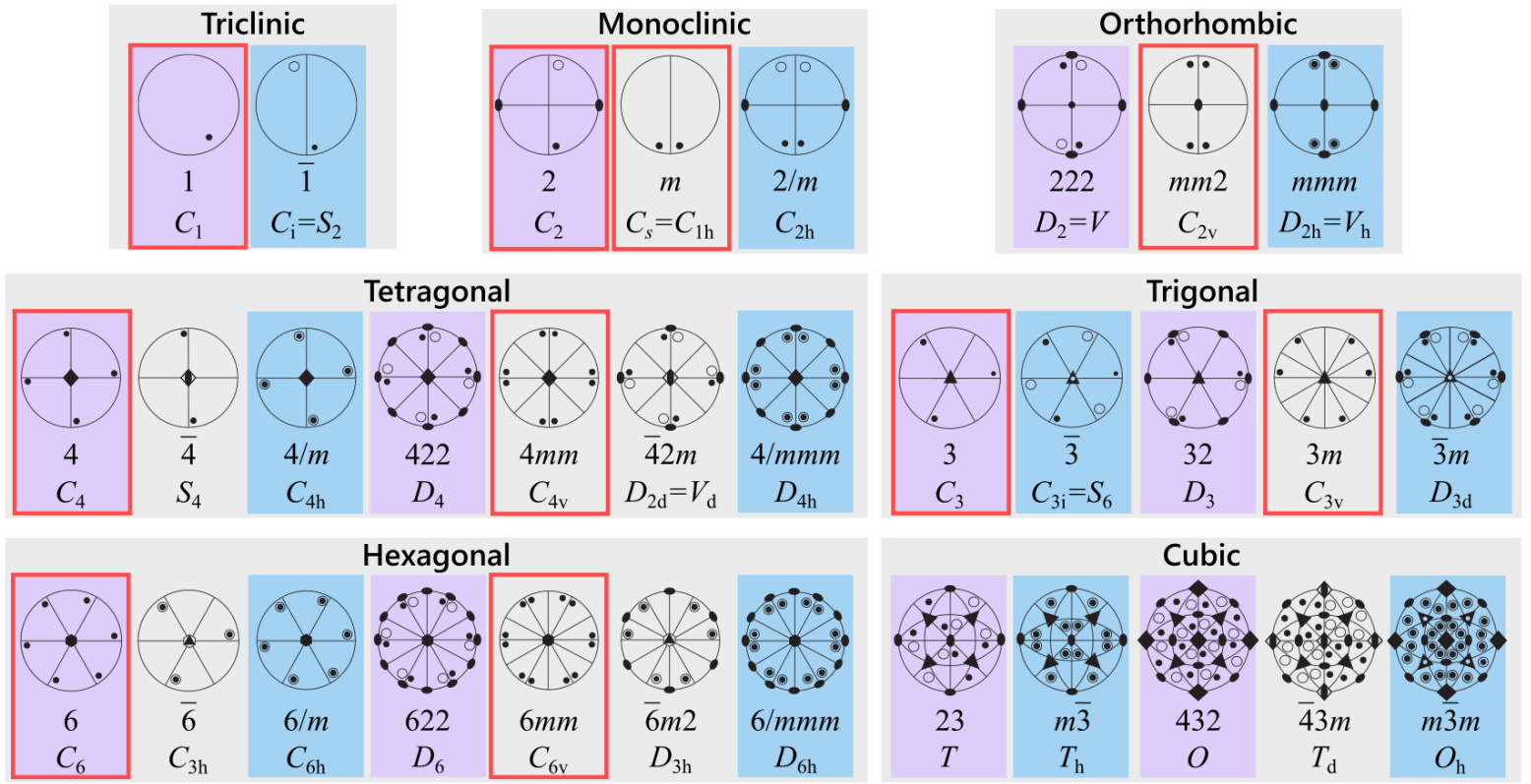
Mirror symmetry



Inversion symmetry



Crystallographic Point Groups



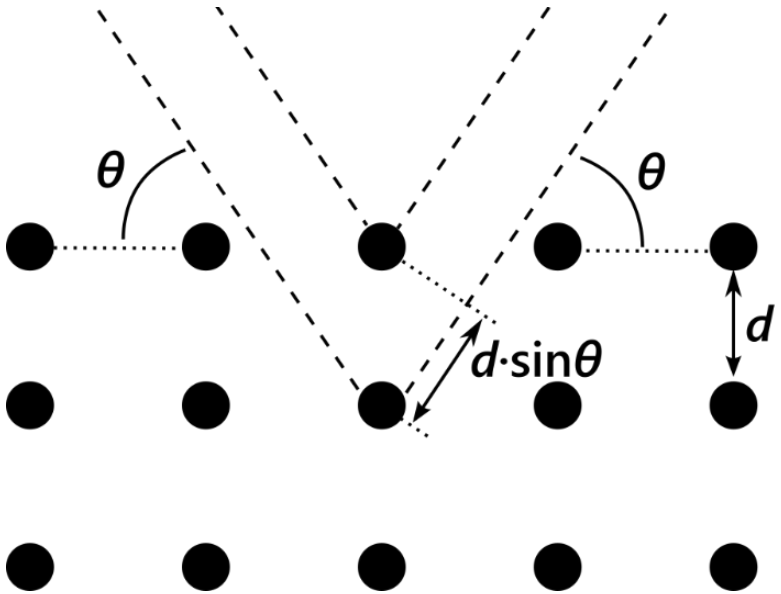
Notation: Hermann-Mauguin / Schönflies

Detailed diagrams: http://pd.chem.ucl.ac.uk/pdnn/symm2/pntgrp1.htm

Centrosymmetric
Enantiomorphic
Polar

Symmetry – So What?

1. Enables identification of materials using scattering techniques

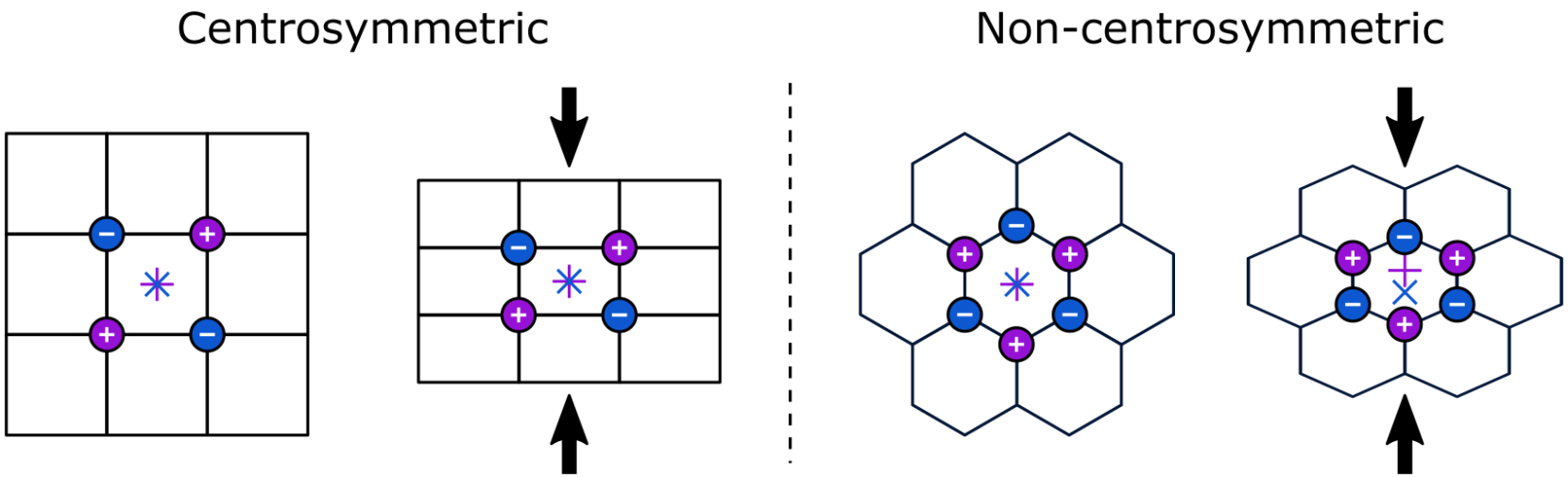


Bragg's law

$2d \sin\theta = n\lambda$

Symmetry – So What?

2. Enables prediction of certain material properties qualitatively



Neumann's Principle

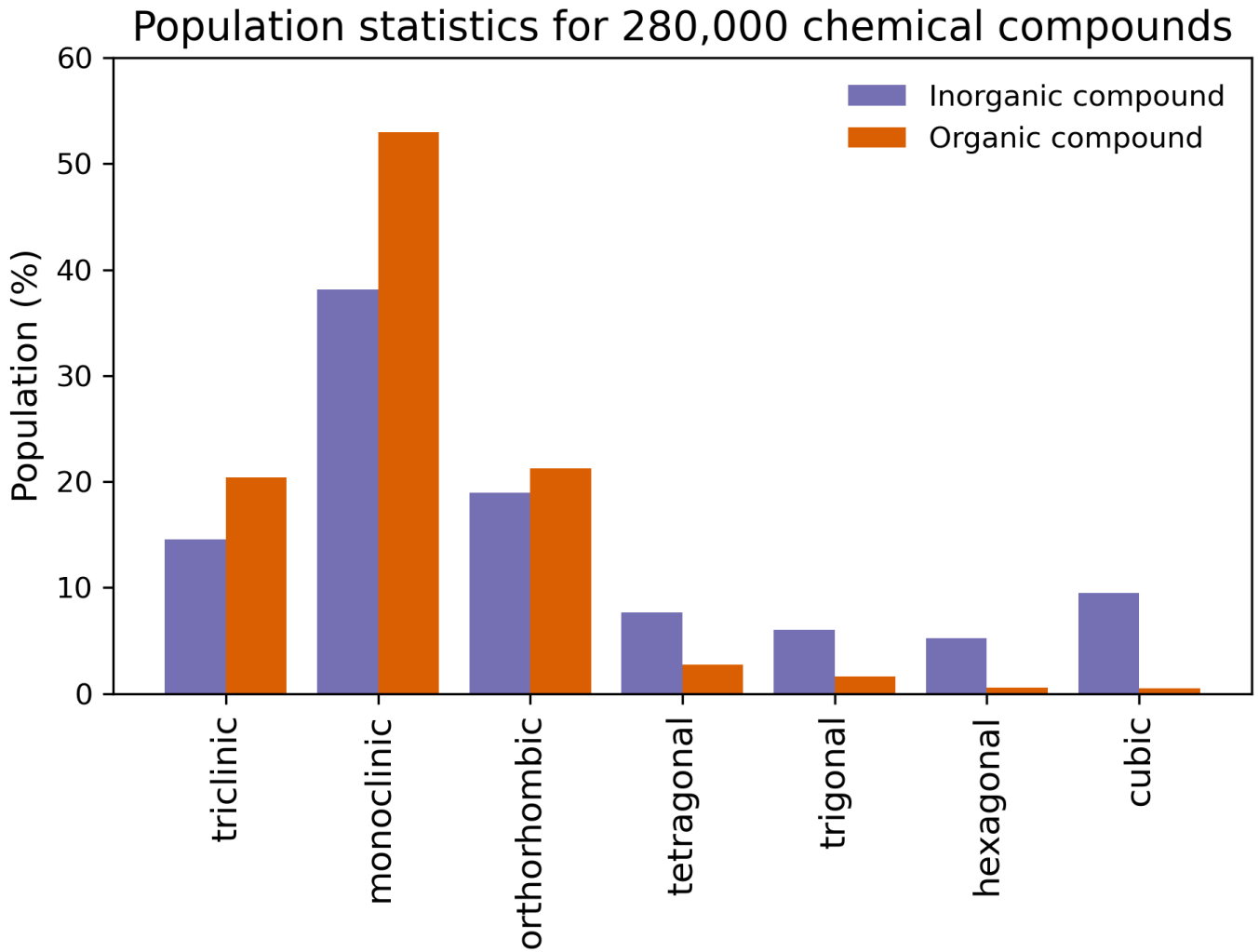
Symmetry of any *physical property* of a crystal must include the *symmetry elements* of its point group

Symmetry – So What?

List of allowed/forbidden properties based on point group symmetry:

Property	Centrosymmetric (with inversion)	Enantiomorphic (chiral, no inversion/mirror)	Polar (unique axis)	Polar + Enantiomorphic
Piezoelectricity	❌ Forbidden	✅ Allowed	✅ Allowed	✅ Allowed
Ferroelectricity	❌ Forbidden	❌ Forbidden	✅ Allowed	✅ Allowed
Pyroelectricity	❌ Forbidden	❌ Forbidden	✅ Allowed	✅ Allowed
Optical activity (chirality)	❌ Forbidden	✅ Allowed	❌ Forbidden	✅ Allowed
Second Harmonic Generation (SHG)	❌ Forbidden	✅ Allowed	✅ Allowed	✅ Allowed

Symmetry in Crystals – Statistics

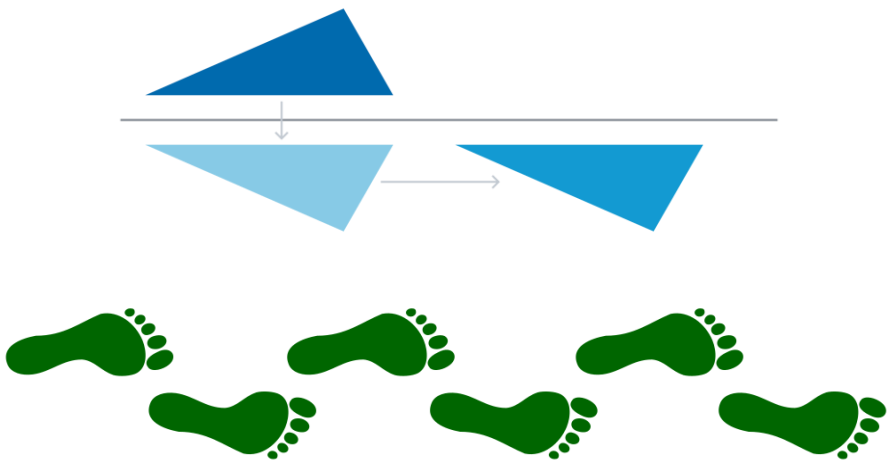


Space Groups

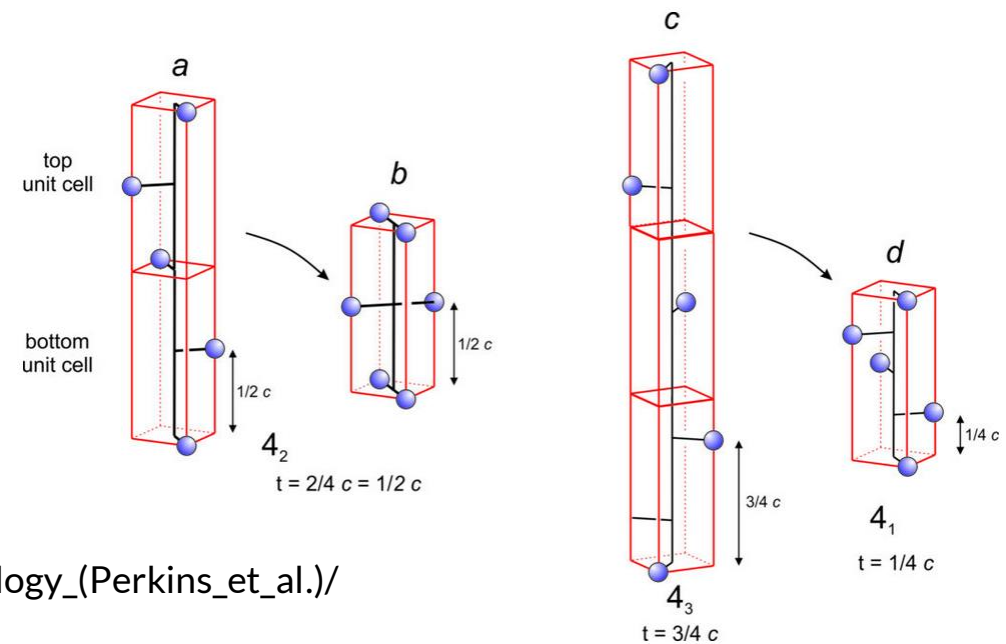
Also considers allowed translations within the lattice (centering types of Bravais lattices)

Adds two symmetry operations:

Glide Plane



Screw Axis



wikipedia.org and https://geo.libretexts.org/Bookshelves/Geology/Mineralogy_(Perkins_et_al.)/

Space Groups

Glide Plane

1. Reflection at a plane
2. Translation (either ½ or ¼)

Possible glide planes:
a → reflection (*a*,*b*) + ½ transl. in *a* direction
b → reflection (*b*,*c*) + ½ transl. in *b* direction
c → reflection (*b*,*c*) + ½ transl. in *c* direction
n → see video*
d → see video*
e → see video*

Screw Axis

n_m screw axis where $m < n$:
1. Rotation by 360°/*n*
2. Translation by *m*/*n* of the unit cell parallel to the screw axis

Possible screw axes:
2_1, 3_1, 4_1, 4_2, 6_1, 6_2, and 6_3
Enantiomorphous ones: 3_2, 4_3, 6_4, 6_5

→ 230 Space groups

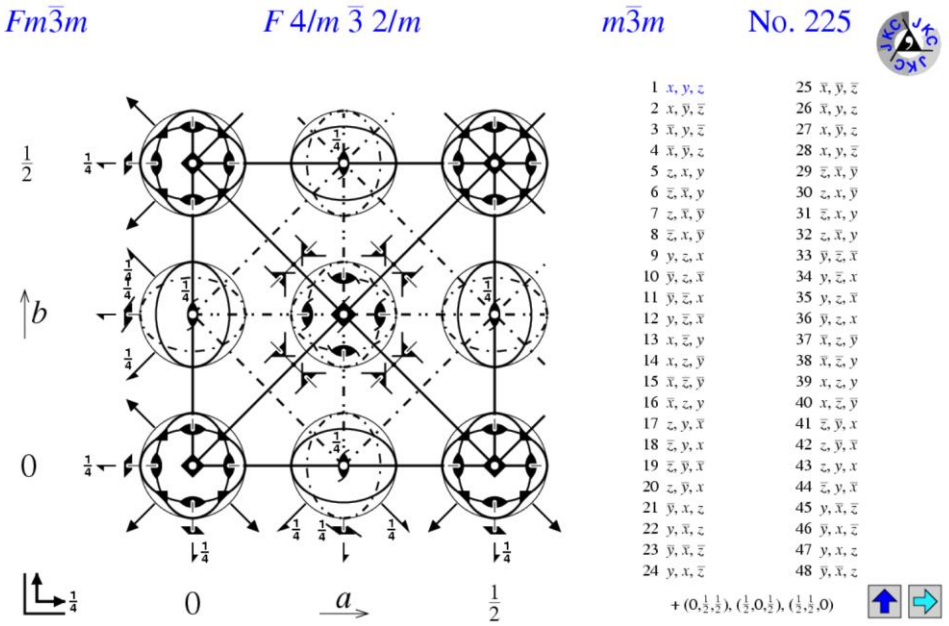
* https://www.youtube.com/watch?v=C8wZdLV6u-4

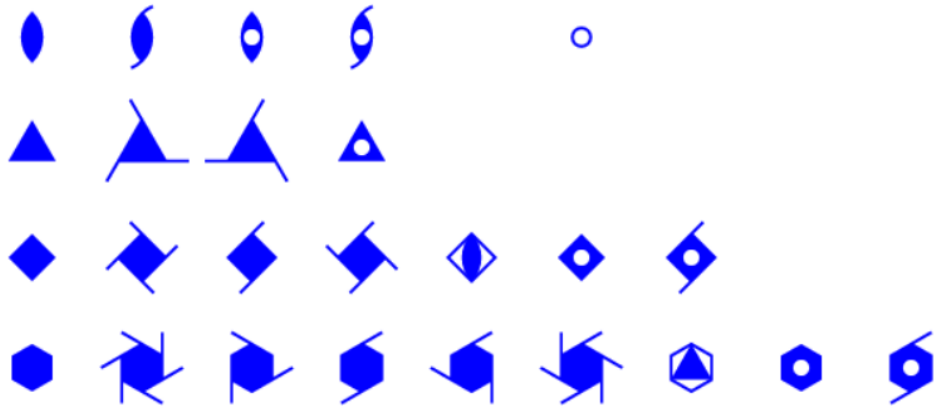
Space Group Diagrams

Symmetry operation symbols:

Full explanation here:
http://img.chem.ucl.ac.uk/sgp/mainmenu.htm

NaCl example:





Crystal family	Crystal system	Required symmetries of the point group	Point groups	Space groups	Bravais lattices	Lattice system
Triclinic	Triclinic	None	2	2	1	Triclinic
Monoclinic	Monoclinic	1 twofold axis of rotation or 1 mirror plane	3	13	2	Monoclinic
Orthorhombic	Orthorhombic	3 twofold axes of rotation or 1 twofold axis of rotation and 2 mirror planes	3	59	4	Orthorhombic
Tetragonal	Tetragonal	1 fourfold axis of rotation	7	68	2	Tetragonal
Hexagonal	Trigonal	1 threefold axis of rotation	5	7	1	Rhombohedral
				18	1	Hexagonal
	Hexagonal	1 sixfold axis of rotation	7	27		
Cubic	Cubic	4 threefold axes of rotation	5	36	3	Cubic
6	7	**Total**	32	230	14	7

Wyckoff Letters/Positions

Describe the sites in a space group with **distinct symmetries**

Of form: number letter (x, y, z)
e.g., 3c (0,½ ,½)

- Number is the multiplicity (how many sites are generated from the single Wyckoff site)
- Letters start from a and increase roughly from high to low symmetry (different for each space group)
- Fractional coordinate of the location in the cell

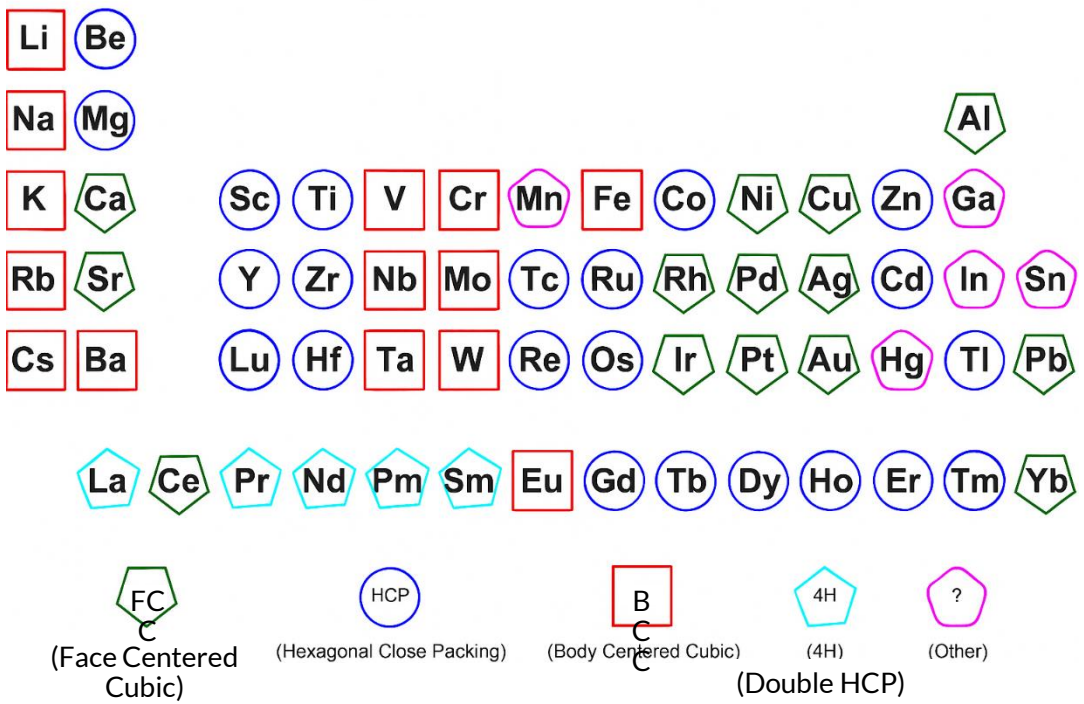
Can be looked up for each space group:
https://www.cryst.ehu.es/cryst/get_wp.html

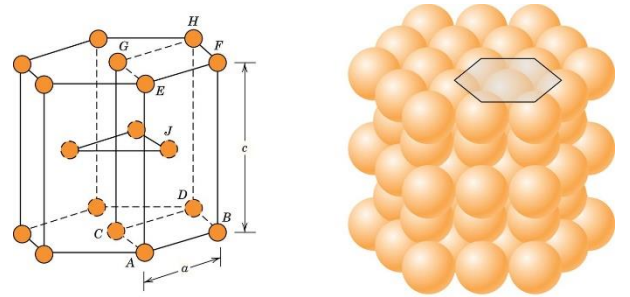
Space Group *Pm*-3 (No. 200)

Multiplicity	Wyckoff letter	Site symmetry	Coordinates
24	l	1	(x,y,z) (-x,-y,z) (-x,y,-z) (x,-y,-z) (z,x,y) (z,-x,-y) (-z,-x,y) (-z,x,-y) (y,z,x) (-y,z,-x) (y,-z,-x) (-y,-z,x) (-x,-y,-z) (x,y,-z) (x,-y,z) (-x,y,z) (-z,-x,-y) (-z,x,y) (z,x,-y) (z,-x,y) (-y,-z,-x) (y,-z,x) (-y,z,x) (y,z,-x)
12	k	m..	(1/2,y,z) (1/2,-y,z) (1/2,y,-z) (1/2,-y,-z) (z,1/2,y) (z,1/2,-y) (-z,1/2,y) (-z,1/2,-y) (y,z,1/2) (-y,z,1/2) (y,-z,1/2) (-y,-z,1/2)
12	j	m..	(0,y,z) (0,-y,z) (0,y,-z) (0,-y,-z) (z,0,y) (z,0,-y) (-z,0,y) (-z,0,-y) (y,z,0) (-y,z,0) (y,-z,0) (-y,-z,0)
8	i	.3.	(x,x,x) (-x,-x,x) (-x,x,-x) (x,-x,-x) (-x,-x,-x) (x,x,-x) (x,-x,x) (-x,x,x)
6	h	mm2 . .	(x,1/2,1/2) (-x,1/2,1/2) (1/2,x,1/2) (1/2,-x,1/2) (1/2,1/2,x) (1/2,1/2,-x)
6	g	mm2 . .	(x,1/2,0) (-x,1/2,0) (0,x,1/2) (0,-x,1/2) (1/2,0,x) (1/2,0,-x)
6	f	mm2 . .	(x,0,1/2) (-x,0,1/2) (1/2,x,0) (1/2,-x,0) (0,1/2,x) (0,1/2,-x)
6	e	mm2 . .	(x,0,0) (-x,0,0) (0,x,0) (0,-x,0) (0,0,x) (0,0,-x)
3	d	mmm . .	(1/2,0,0) (0,1/2,0) (0,0,1/2)
3	c	mmm . .	(0,1/2,1/2) (1/2,0,1/2) (1/2,1/2,0)
1	b	m-3.	(1/2,1/2,1/2)
1	a	m-3.	(0,0,0)

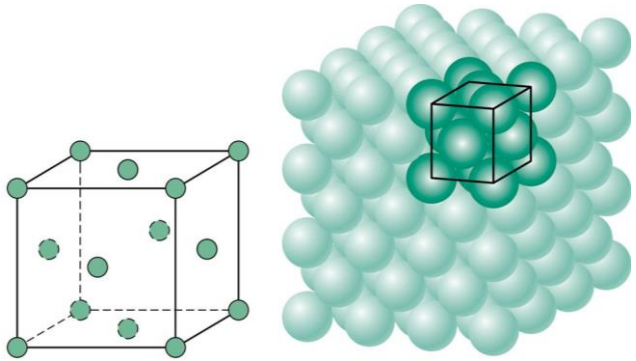
Close-Packed Crystal Structures

Elemental metals (and nobel gases at low T) like to closely pack





Hexagonal Closed Packed (HCP)



Face-Centered Cubic (FCC)

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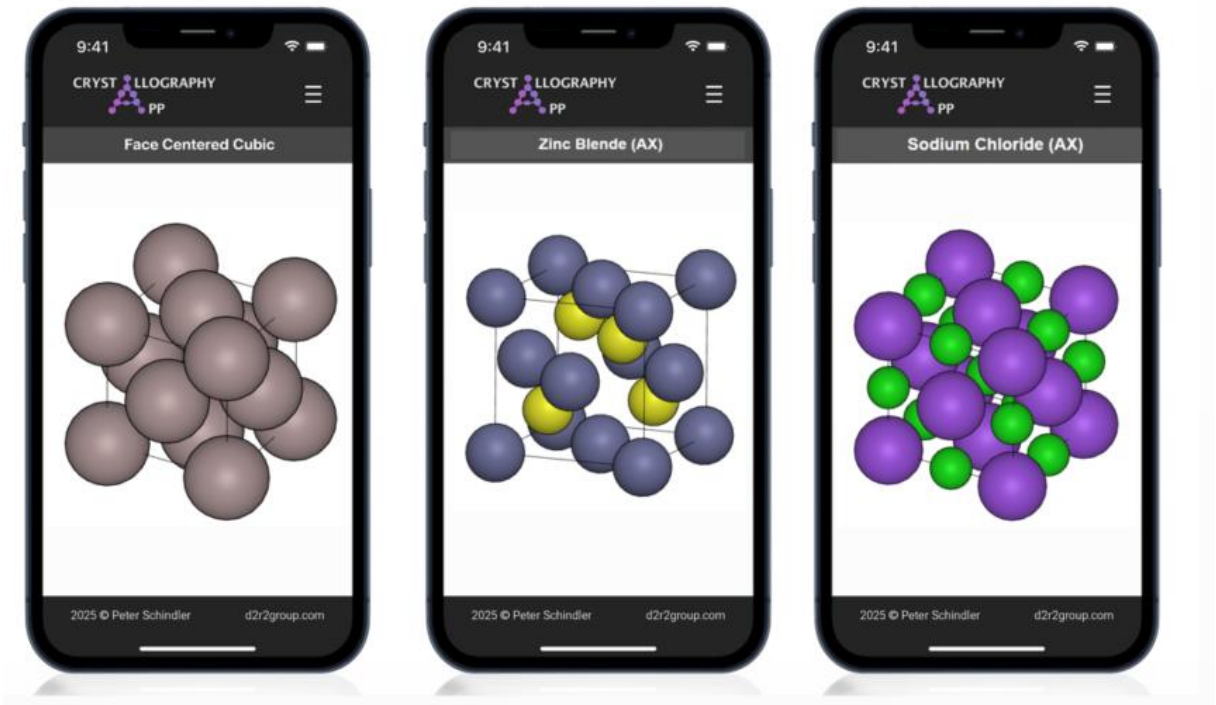
Ceramic and Other Common Crystal Structures

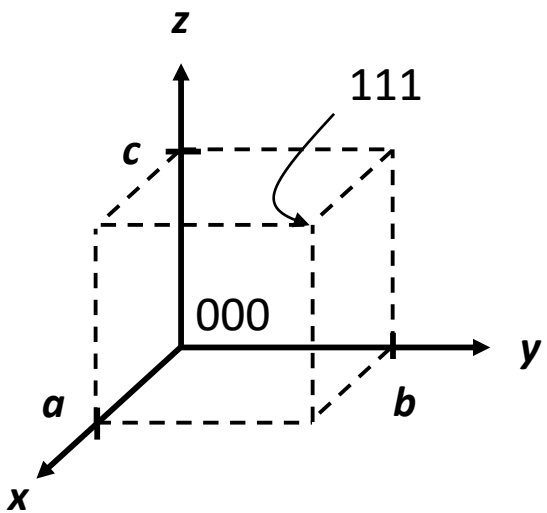
There are a few common crystal structure prototypes for binary ceramics.



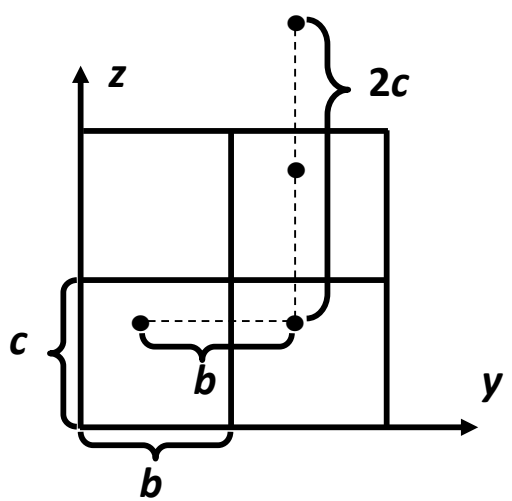
crystallography.app

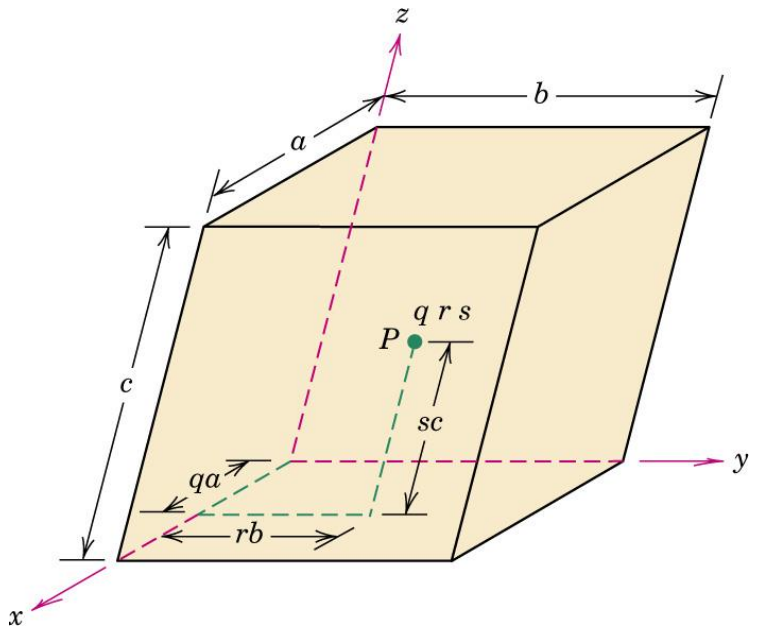
Fractional Coordinates in Lattices

- ***q r s*** represent the coordinates at point *P*
- The fraction of the lattice parameter (distance) along each axis is given by ***q r s***
- Written **without any parentheses**



Point coordinates:
Center of the unit cell: ½ ½ ½
One corner of the unit cell: 111





Invariance to translation:

Integer multiples of lattice constants
→ *identical position* in repeating unit cell

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Metric Tensor and Distances in Lattices

Metric tensor for lattice with unit cell vectors $\{\vec{e}_i\} = \{\vec{a}, \vec{b}, \vec{c}\}$

$$g_{ij} = \vec{e}_i \cdot \vec{e}_j \qquad g = \begin{pmatrix} \vec{a}^2 & \vec{a}\cdot\vec{b} & \vec{a}\cdot\vec{c} \\ \vec{b}\cdot\vec{a} & \vec{b}^2 & \vec{b}\cdot\vec{c} \\ \vec{c}\cdot\vec{a} & \vec{c}\cdot\vec{b} & \vec{c}^2 \end{pmatrix}$$

Can be used to convert fractional to Cartesian coordinates (and vice versa with the inverse metric tensor, g^{-1})

$$x^i_{\text{cart}} = g_{ij} x^j_{\text{frac}} \qquad \vec{x}_{\text{cart}} = g \cdot \vec{x}_{\text{frac}}$$

Also used as a norm to get the distance in a lattice (e.g., distance between two atomic sites $\vec{v} = \vec{x}_1 - \vec{x}_2$):

$$d = g_{ij} v^i_{\text{frac}} v^j_{\text{frac}} \qquad d = v_{\text{frac}} \cdot g \cdot v_{\text{frac}}$$

Things we Didn't Cover

- Packing density calculations [cf. undergrad. MatSci course*]
- Coordination number, number of nearest neighbors [cf. undergrad. MatSci course*]
- Details on ceramic crystal structures [cf. undergrad. MatSci course*]
- Crystallographic directions [cf. undergrad. MatSci course*]
- Crystallographic planes (Miller indices) [cf. undergrad. MatSci course*]
- Reciprocal lattice and reciprocal metric tensor [will cover during DFT]
- *Few more advanced concepts*: Magnetic space groups, laue classes, …

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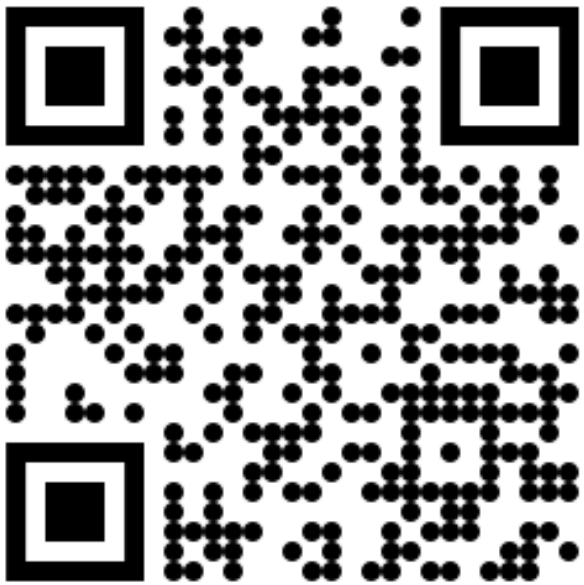
Lecture Feedback



Please, scan the QR code and take a minute to let me know how the lecture was and mention any **feedback/questions**

This form is **anonymous!**