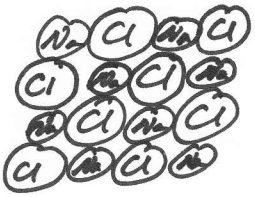
Descriptive Crystal Structures

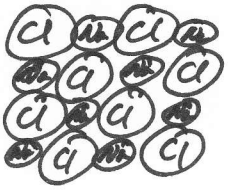
Drawing / visualizing 3-dimensional structures can be very difficult → many 3-d crystal drawers / visualizers available online. 2-d representations take some practice and artistic skill.

Symmetry: previously we've worked w/ point groups
↳ rotational, reflection, inversion etc.
↳ defined by point, axis, or plane.

For extended structures (solids, crystals) we are interested in also looking at translational symmetry.

Consider NaCl:

1st layer: 

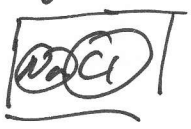
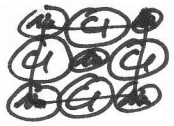
2nd layer: 

3rd layer: same as first.

4th layer: same as 2nd

⋮

Identify repeating unit:

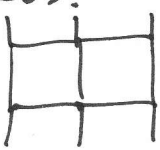
 or 

we usually pick this one

unit cell: can describe entire crystal structure by just translating by 1 unit cell at a time

↙

no rotations or other symmetry operations to close pack unit cells. (no voids)

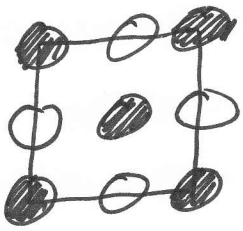


vs.

actually

void

In recognition of the unit cell, we can also draw them like this:



● = Na: 0, 1
Cl: $\frac{1}{2}$

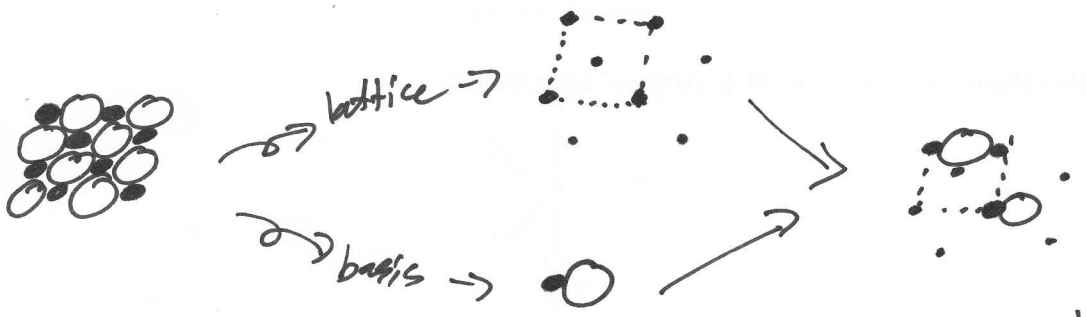
○ = Na: $\frac{1}{2}$
Cl: 0, 1

↖ specify z height w/in unit cell length 1.

How to describe this structure more generally to group them w/ other similar structures?

Lattice and Basis.

Na: ●
Cl = ○



you can put the basis @ any point in the lattice to get the same structure (i.e. all lattice pts. are identical).

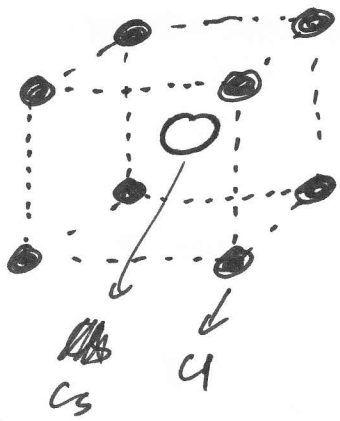
→ lattice: FCC
face-centered-cubic

basis: Na (0, 0, 0)
Cl ($\frac{1}{2}$, 0, 0)
↳ x, y, z w/in unit cell.

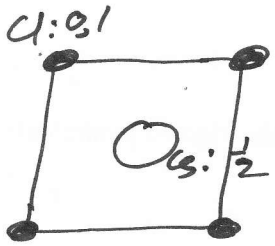
Each unit cell should only contain 1 basis total (for primitive lattices).

→ note: FCC is not a primitive lattice.
total basis > 1.

Examples: CsCl



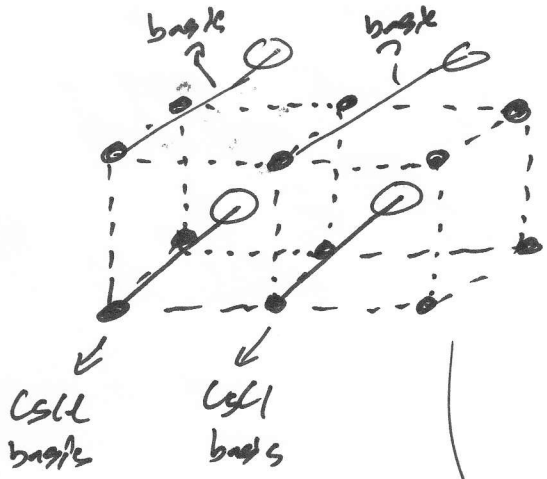
or



What is the lattice and basis? Not bcc!

Simple cubic, basis = Cs $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$
Cl $(0,0,0)$

or could also be Cs $(0,0,0)$ Cl $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ for different unit cell drawing.



Simple cubic = primitive cell, 1 basis per unit cell.

to take note of edge sharing and vertex/face sharing

→ each vertex shared amongst 8 unit cells.

per unit cell: $8 \times \frac{1}{8} = 1$ Cl
(8 vertices, ⅛ sharing)

$+ \quad 1$ Cs

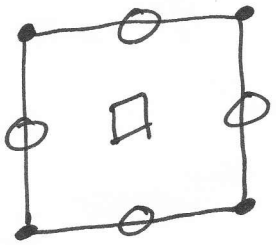
1 CsCl

Example: perovskites: ABX_3

↑ ↑ ↳ anion.

cation diff. cation

$BaTiO_3$



○ = O: (½)

● = Ba (0,1)

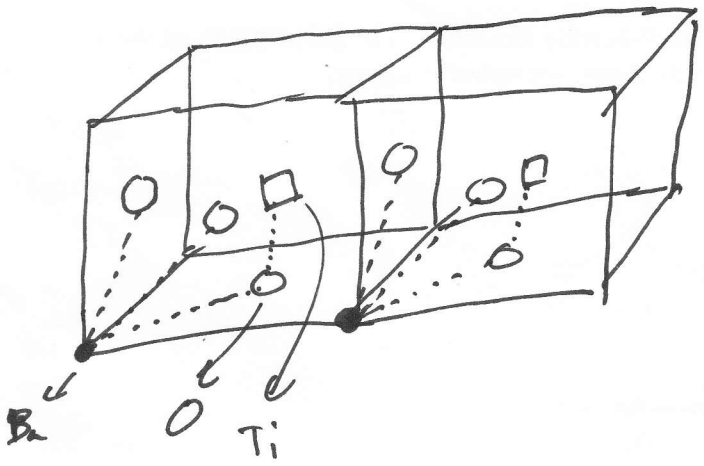
□ = Ti (½)

○: (0,1)

Ba = vertex

○ = face

Ti = body



Simple cubic: Ba (0,0,0)

O (½,0,0)

(0,½,0)

(0,0,½)

Ti (½,½,½)

per unit cell: $BaTiO_3$.

Example: Silicon.

↳ each Si tetrahedrally coordinated.

same structure as diamond.

FCC: Basis Si (0,0,0)

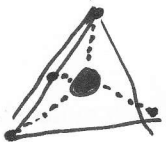
(¼,¼,¼)

Can think of it as one Si FCC lattice + another Si FCC lattice offset by (¼,¼,¼).

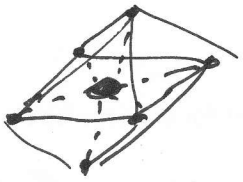
See physical model, or use online 3-d visualizer.

We can also describe these structures based on hole filling.

Generally, two types of holes to fill:



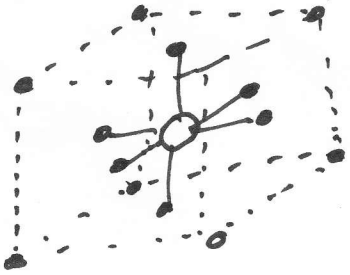
4-coordinate tetrahedral



6-coordinate octahedral

NaCl:

FCC Na structure, fill all the octahedral holes. w/ Cl.



Si:

FCC Si structure: fill $\frac{1}{2}$ of tetrahedral holes w. Si.