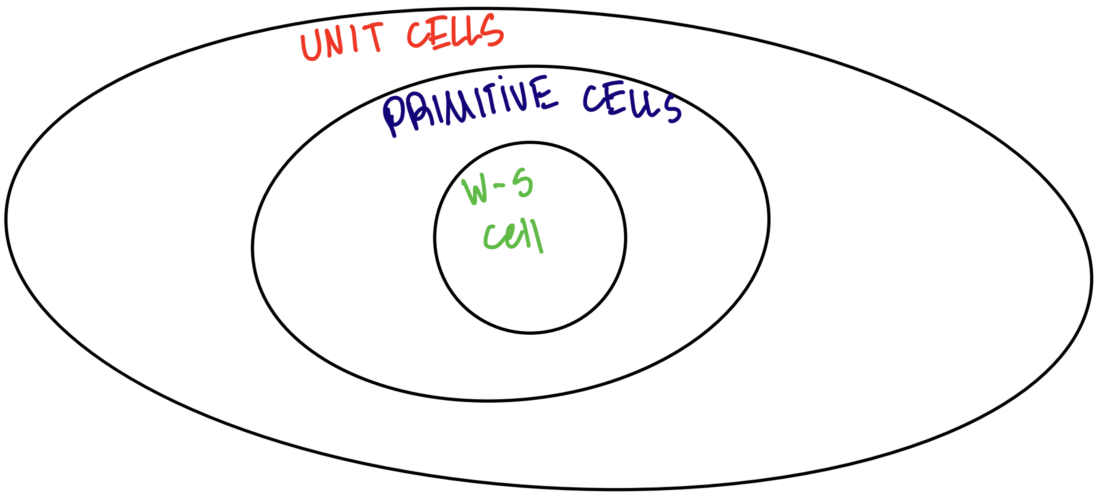
Phys 425

Lecture 2.

for our heirarchy,
- we have unit cells
  ↳ primitive cells → Wigner - Seitz (unit cell)

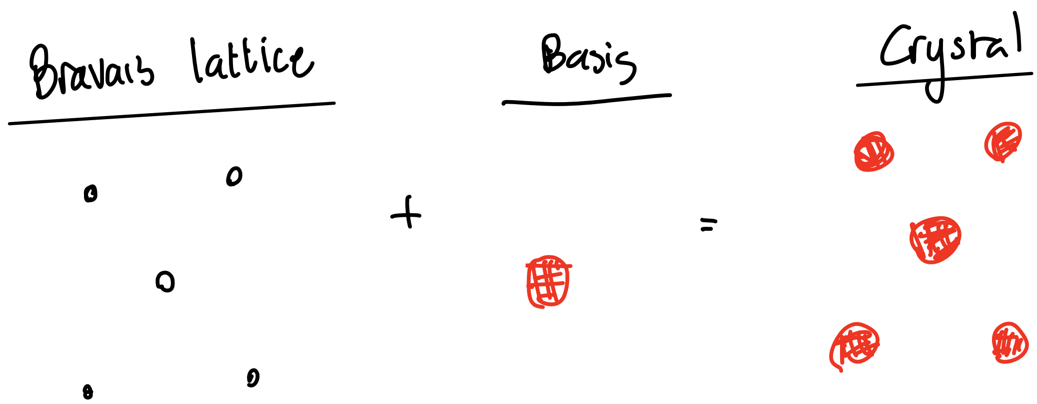


The Bravais lattice is the blueprint of a real crystal.

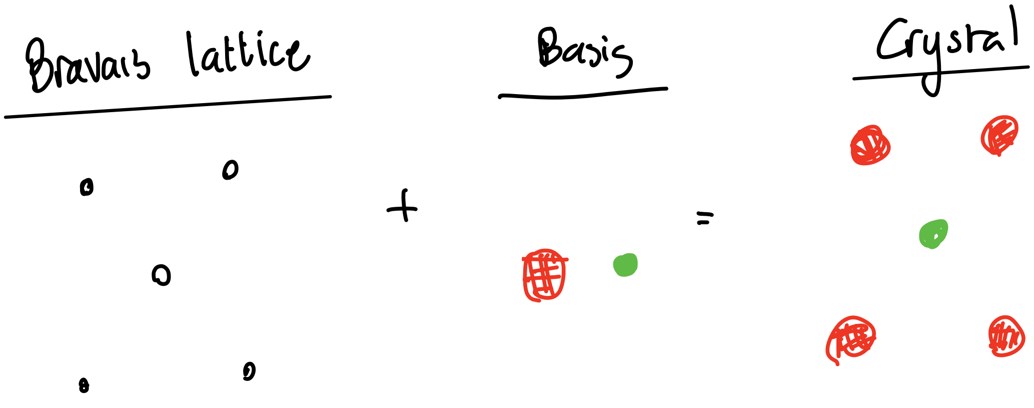
↳ to get a real crystal, we need to provide a "basis."

is not restricted in the # of atom types

eg



Or use two atoms for basis



Every crystal needs 2 things

1. A lattice (we use Bravais)
2. A basis

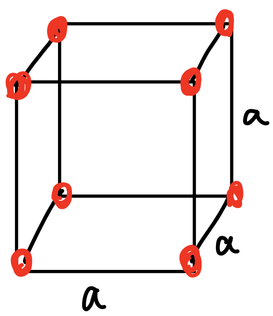
3D Crystals:

Most solids have one of three lattice structures.

most simple one →

1. Simple cubic (SC) -
2. Body - Centered Cubic (BCC)
3. Face - Centered Cubic (FCC)

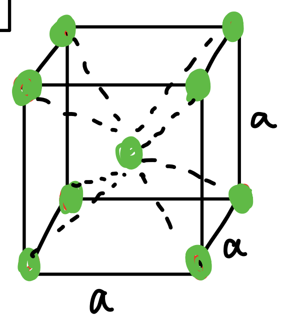
SC:



all locations at length $\underline{a}$ from somewhere

$$\boxed{\text{basis: } a(0,0,0) \ \underline{\text{or}} \ a\left(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2}\right)}$$

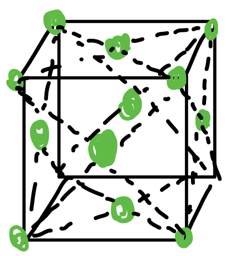
BCC: atom in center of cube body



1/2 in every axis, so

$\boxed{\text{Basis} = a(0,0,0) \text{ and } a(\tfrac{1}{2},\tfrac{1}{2},\tfrac{1}{2})}$

FCC: Every face has an atom at the center



Basis: $a(0,0,0)$ and $a(\tfrac{1}{2},\tfrac{1}{2},0)$ and $a(\tfrac{1}{2},0,\tfrac{1}{2})$ and $a(0,\tfrac{1}{2},\tfrac{1}{2})$

Coordination # (Z) = how many nearest neighbors you have,
how many atoms you have in your unit cell.

	Coordination Number (Z)	Atom / unit cell
SC:	6 (every corner = 3)	1
BCC:	8	2
FCC:	12	4

Crystals prefer tighter packing (more efficient use of space to minimize energy), so it's usually never SC.

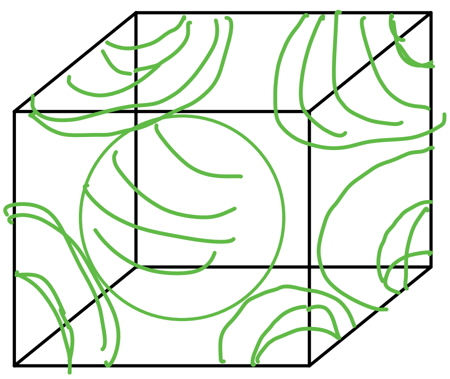
$\hookrightarrow$ prefer higher Atomic Packing Function (APF)

$$\boxed{APF = \frac{(\#\,\text{atoms}/\text{cell}) \times (\text{Vol}/\text{atom})}{(\text{Volume of unit cell})}}$$

— or —

$$\boxed{APF = \frac{N_{atoms}\, V_{atom}}{V_{cell}}}$$

Example BCC:



Each corner atom makes contact with/ central atom.

a. Each atom is rad r

$$l = \sqrt{3}a = 4r$$

$$\Rightarrow a = \frac{4r}{\sqrt{3}}$$

$$APF = \frac{\overset{\#\text{ of atoms}}{2} \times \overbrace{\frac{4}{3}\pi r^3}^{V_{atom}}}{\underbrace{\left(\frac{4r}{\sqrt{3}}\right)^3}_{a^3 = V_{cell}}} = \frac{\pi\sqrt{3}}{8}$$

Reciprocal lattice:

So far we've seen real space lattices.

↳ it's more convenient to do math in the reciprocal space, which is represented by the frequency of distances (wave # (k)) with lattices in wavenumbers

$$k = \frac{2\pi}{a}$$

- so we'll transform to a different lattice.

Given: a lattice point in real space

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

the point

$$\vec{G} = m_1\vec{b}_1 + m_2\vec{b}_2 + m_3\vec{b}_3$$

is in the reciprocal lattice if $e^{i\vec{G}\cdot\vec{R}} = 1$

or ⇒ $$\vec{G}\cdot\vec{R} = 2\pi n$$

for all points in the real lattice.

Note: we that $\vec{G}$ also forms a Bravais lattice if $\vec{R}$ is a Bravais lattice.

$\vec{G}$ is made up of the following reciprocal lattice vectors

$$\vec{b}_1 = \frac{2\pi\, \vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = \frac{2\pi\, \vec{a}_3 \times \vec{a}_1}{\vec{a}_1 (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = \frac{2\pi (\vec{a}_1 \times \vec{a}_2)}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

Check: $\vec{a}_i \cdot \vec{b}_i = 2\pi \delta_{ij}$

Kronecker delta: $\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$