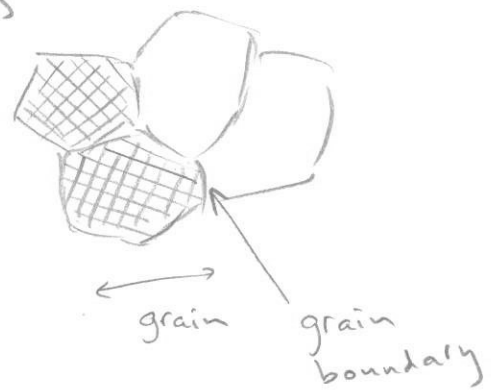
Lecture #3 Crystal lattices

Condensed matter

- Liquids
  - Liquid crystals
  - Short range order
- Solid state
  - Amorphous Glassy
  - Crystalline
    - Polycrystals
    - Monocrystals



Most metals and other solids are crystalline

How to construct a crystal? Start with a Bravaislattice

Bravaislattice – Definition

- × Periodic array of points, infinite
- × Appearing exactly the same from any point

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

$n_i = 0, \pm 1, \pm 2, \ldots$

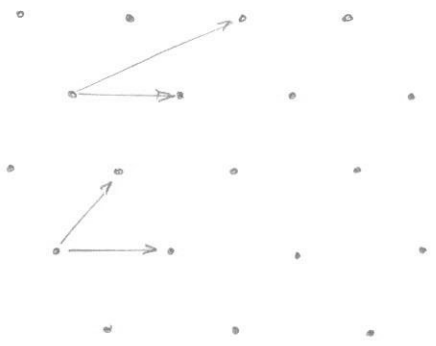
$\bar{a}_i$ = primitive vectors not in same plane

Add a unit of one or more ions at each point → "Basis"

$\Longrightarrow$ Crystal structure

Ex

not a Bravaislattice



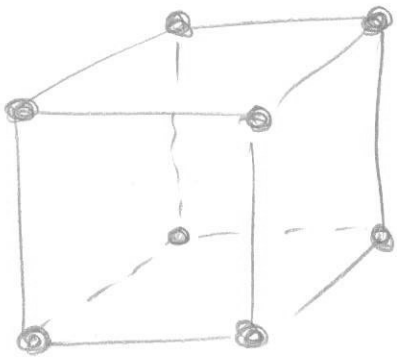
Bravais lattice

- × not parallel primitive vectors
- × All points are reached using primitive vectors

Primitive unit cell — Placed on each B.L. point to fill space, Contains 1 B.L. point

Conventional unit cell — Placed on a subset of a B.L. to fill space. May contain > 1 B.L. point.

Ex. fcc, bcc



Simple cubic (S.C.) unit cell

How to count atoms in a cell, or primitive lattice points in a conventional unit cell?

	Weight
× Corner points	1/8
× Edge points	1/4
× Surface points	1/2
× Inside	1

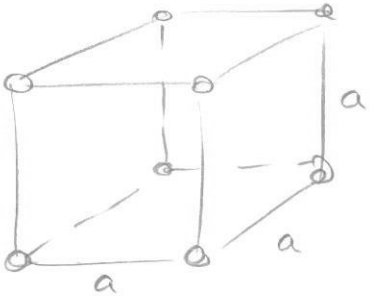
$\Longrightarrow$ SC Contains $8 \times \frac{1}{8} = 1$ lattice point/cell

$\Longrightarrow$ primitive unit cell

Coordination number: number of nearest neighbors of a given lattice point

lattice parameters: Length of lattice vectors $\bar{a}_i$

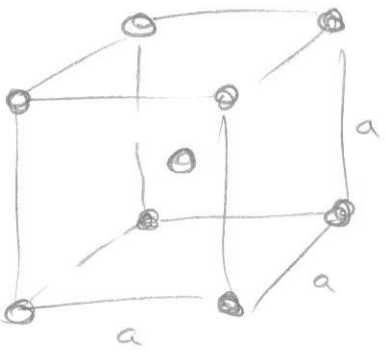
Cubic structures



Simple cubic (sc)

1 lattice point/cell

Coordination number: 6

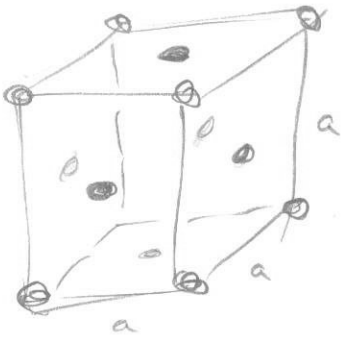


body centered cubic (bcc)

$1 + 8 \times \frac{1}{8} = 2$ lattice points/cell

not primitive cells

coord. number: 8



face centered cubic (fcc)

$8 \times \frac{1}{8} + 6 \times \frac{1}{2} =$

$= 4$ lattice points/cell

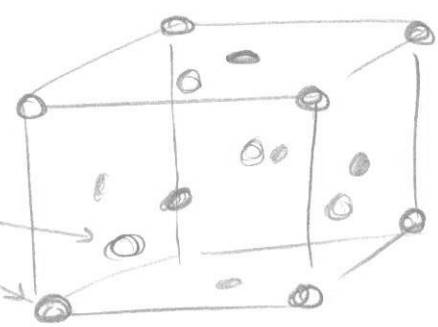
Coordination number: 12

However: Both bcc and fcc are also Bravais lattices

(see p. 67)

Diamond structure: (not a Bravais lattice)

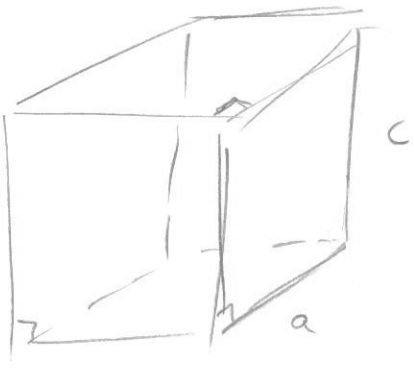
looks like fcc lattice with basis $\bar{0}$ and $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$



these points do not see the same environment (unless rotation)

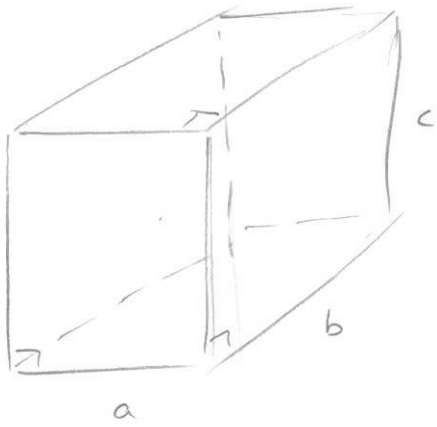
$4 + 4 \times 1 = 8$ lattice pts/cell

(p. 76)



tetragonal:

$c \neq a$

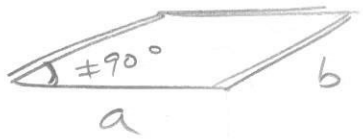


orthorhombic:

$a \neq b \neq c$

Monoclinic:

$a \neq b \neq c$



seen from c-axis direction

Triclinic:

$a \neq b \neq c$

Lattice of minimum symmetry

no angles 90°

Rhombohedral / trigonal:

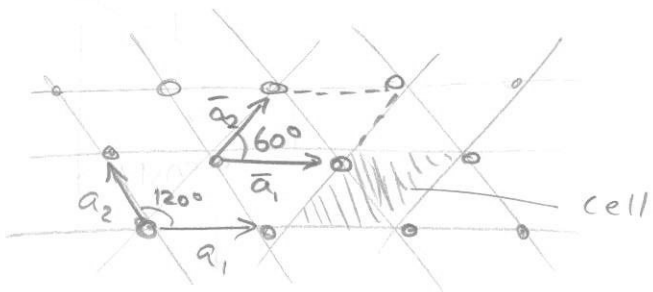
$a = b = c$, equal angles, no special values

Hexagonal:

$a = b$

$\parallel \quad \parallel$

$|\bar{a}_1| \quad |\bar{a}_2|$



c perpendicular to hexagonal plane

Simple hexagonal: Bravaislattice

Hexagonal close-packed (hcp): sh + basis of 2 points

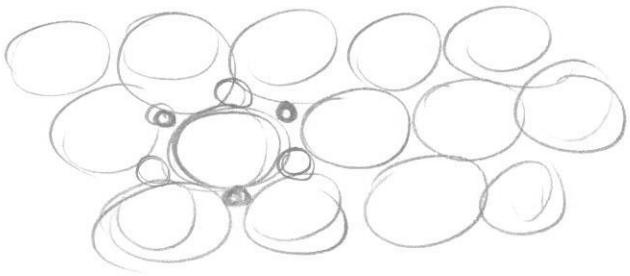
Close-packing

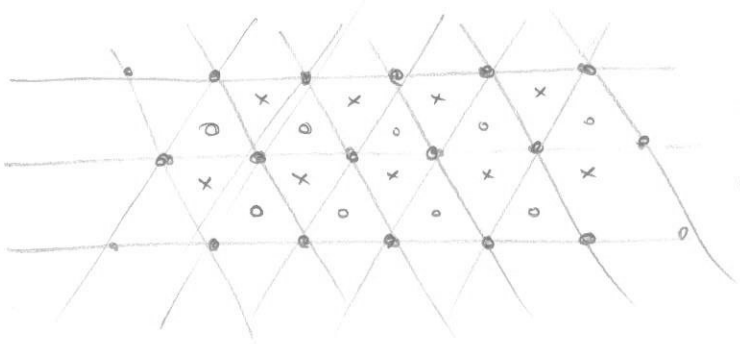
Structures that pack spheres with highest possible density

× hcp hexagonal close packing

ideal if $c = \sqrt{\frac{8}{3}} \cdot a$

× fcc face centered cubic





• 1:st layer "A"

o 2nd layer "B"

× 3rd layer "C"

fcc: A B C A B C ...

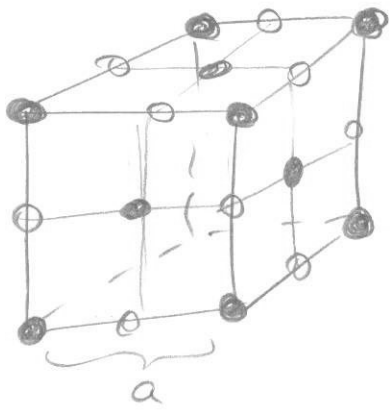
hcp: A B A B

certain rare-earth metal: A B A C A B A C ...

Lithium: A B A B C B C A C ... at T < 70K

Bases with different type of ions

Sodium chloride



fcc + basis $\bar{O}$ and $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

$\bar{O}$ — Na

$\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$ — Cl

Cesium chloride : s.c + basis $\bar{O}$ and $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

Cs — $\bar{O}$

Cl — $\frac{a}{2}(\hat{x}+\hat{y}+\hat{z})$

Zincblende : fcc + basis $\bar{O}$ and $\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$

"diamond lattice"

$\bar{O}$ — Zn

$\frac{a}{4}(\hat{x}+\hat{y}+\hat{z})$ — S

(Ch. 7) 14 Bravais lattices (5 2D-B.L.) divided into 7 crystal systems

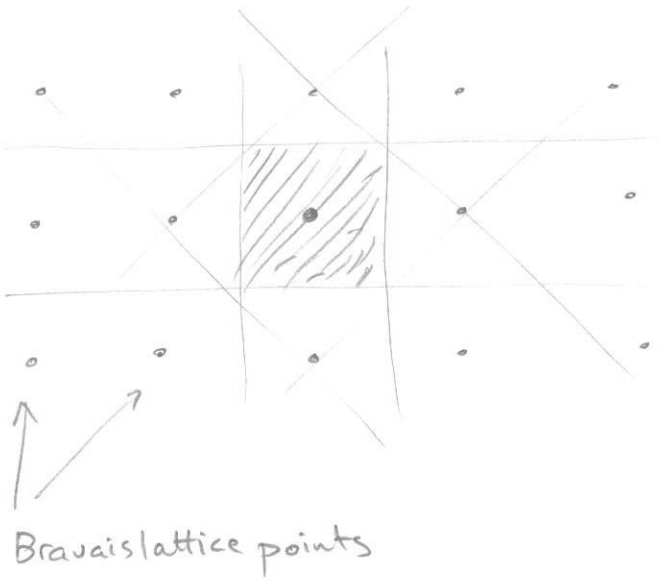
3	cubic (sc, fcc, bcc)	
2	tetragonal	
4	orthorhombic	
2	monoclinic	
1	triclinic	
1	trigonal	
1	hexagonal (simple hexagonal)	
Σ 14		

Add basis ⇓ 230 space groups (possible symmetries)

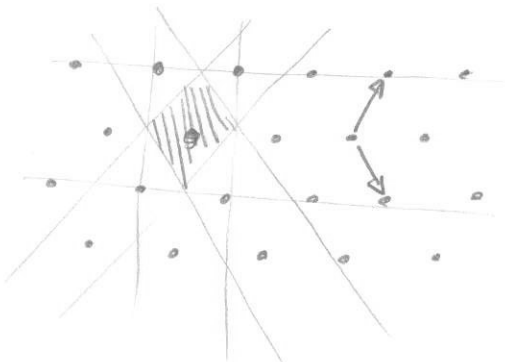
Wigner - Seitz cell

Def: Primitive unit cell containing the space closer to its cell center than to the cell center of any other neighboring cell.

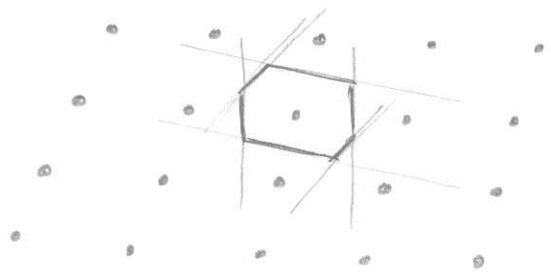
Construction: Bisect distances to neigboring points



cubic



hexagonal



Structure

Examples : sc : Po

bcc : Li, Na, K, Ta, V, Nb, W

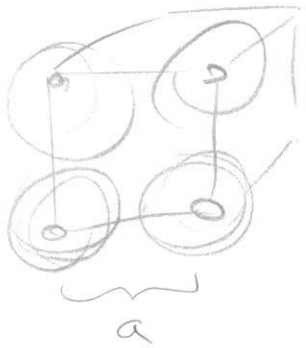
fcc : Ar, Ne, Cu, Ag, Au, Pd, Pt
Al, Ni, Rh

hcp : Cd, Mg, He, Be, Ti, Zn, Zr,
Co, Gd

diamond : diamond, Si, Ge

Ex Calculate packing density for sc, bcc, fcc

sc



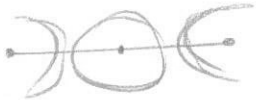
$2r = a$

$$f = \frac{8 \cdot \frac{1}{8} \cdot \frac{4}{3}\pi r^3}{a^3} = \frac{\frac{4}{3}\pi r^3}{(2r)^3} = \frac{\pi}{6} \approx 52\%$$

(volume of "balls" / volume of cell)

bcc

Diagonal:



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

$$f = \frac{2 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{3}}\right)^3} = \frac{\sqrt{3}\pi}{8} \approx 68\%$$

fcc

Surface diagonal:

$4r = \sqrt{2} \cdot a$

$$f = \frac{4 \cdot \frac{4}{3}\pi r^3}{\left(\frac{4r}{\sqrt{2}}\right)^3} = \frac{\sqrt{2}\pi}{6} \approx 74\%$$

Closepacked