**(Primitive)**
*Cubic*

- e.g. Mn
- Space group: I-43m (SG number: 217)
- Mn Structure: cubic
- Cell parameters:
  - $a$: 891.25 pm
  - $b$: 891.25 pm
  - $c$: 891.25 pm
  - $\alpha$: 90.000°
  - $\beta$: 90.000°
  - $\gamma$: 90.000°
Body Centred Cubic (BCC)

- e.g. \( \alpha \)-Fe, V, Cr, Mo, W
- Space group: Im-3m (SG number: 229)
- Fe Structure: bcc (body-centred cubic)
- Cell parameters:
  - \( a \): 286.65 pm
  - \( b \): 286.65 pm
  - \( c \): 286.65 pm
  - \( \alpha \): 90.000°
  - \( \beta \): 90.000°
  - \( \gamma \): 90.000°
Face Centred Cubic (FCC)

- e.g. $\gamma$-Fe, Al, Ni, Cu, Ag, Pt, Au
- Space group: Fm-3m (SG number: 225)
- Al Structure: ccp (cubic close-packed)
- Cell parameters:
  - $a$: 404.95 pm
  - $b$: 404.95 pm
  - $c$: 404.95 pm
  - $\alpha$: 90.000°
  - $\beta$: 90.000°
  - $\gamma$: 90.000°
Hexagonal Close Packed (HCP)

- e.g. Be, Mg, $\alpha$-Ti, Zn, Zr
- Space group: P63/mmc
- (SG number: 194)
- Zn Structure: hcp
- Cell parameters:
  - $a$: 266.49 pm
  - $b$: 266.49 pm
  - $c$: 494.68 pm
  - $\alpha$: 90.000°
  - $\beta$: 90.000°
  - $\gamma$: 120.000°
HCP Unit cell – plan view

$\mathbf{r}_{at}$
HCP Unit cell – side view

C/2

$r_{at}$
HCP reduced sphere view
Close Packing  FCC vs. HCP

(a) Stacking of close packed planes

(b) Stacking of close packed planes

(c) Face-centered cubic

(d) Hexagonal close packed
Caesium chloride

- (Primitive) cubic
Sodium chloride

FCC

2 ions per lattice point

(a)

(b)

(c)
Cristobalite  

- e.g. $\text{SiO}_2$
Diamond cubic (FCC)

- e.g. Si, Ge, grey-Sn
Zinc blende (FCC)

- e.g. GaAs, AlP, InSb (III-V SCs)
- ZnS, CdS, HgTe (II-VI SCs)
Wurtzite (Hexagonal)

- e.g. ZnS, ZnO, CdS
Carbon polymorphism

- Graphite
Carbon polymorphism

- Buckminster Fullerene C60
- Carbon nanotube
The density of a crystalline material can be calculated by

\[ \rho = \frac{n \cdot \text{atomic mass}}{V_{\text{Unit Cell}}} \]

or

\[ \rho = \frac{n \cdot \text{atomic weight}}{N_A \cdot V_{\text{Unit Cell}}} \]
Imperfections

- Point defects
Lattice strains

Tensile

Compressive
Notice lattice strains

- Point defects
Number of Defects

- Number of vacancies \((N_V)\) is given by

\[
N_V = N_0 e^{-E_a / kT}
\]

where \(N_0\) is number of atomic sites and \(E_a\) is the activation energy for the formation of a vacancy.
Edge Dislocation
Perfect Crystal
Edge Dislocation
Burgers Vector

- The vector necessary to complete ‘close’ a path ‘surrounding’ the dislocation.
Edge Dislocation Motion
Screw Dislocation viewed from above

Dislocation along line AB

open circles: atoms above slip plane
closed circles: atoms below slip plane