PY2N20
Material Properties and Phase Diagrams
Lecture 2

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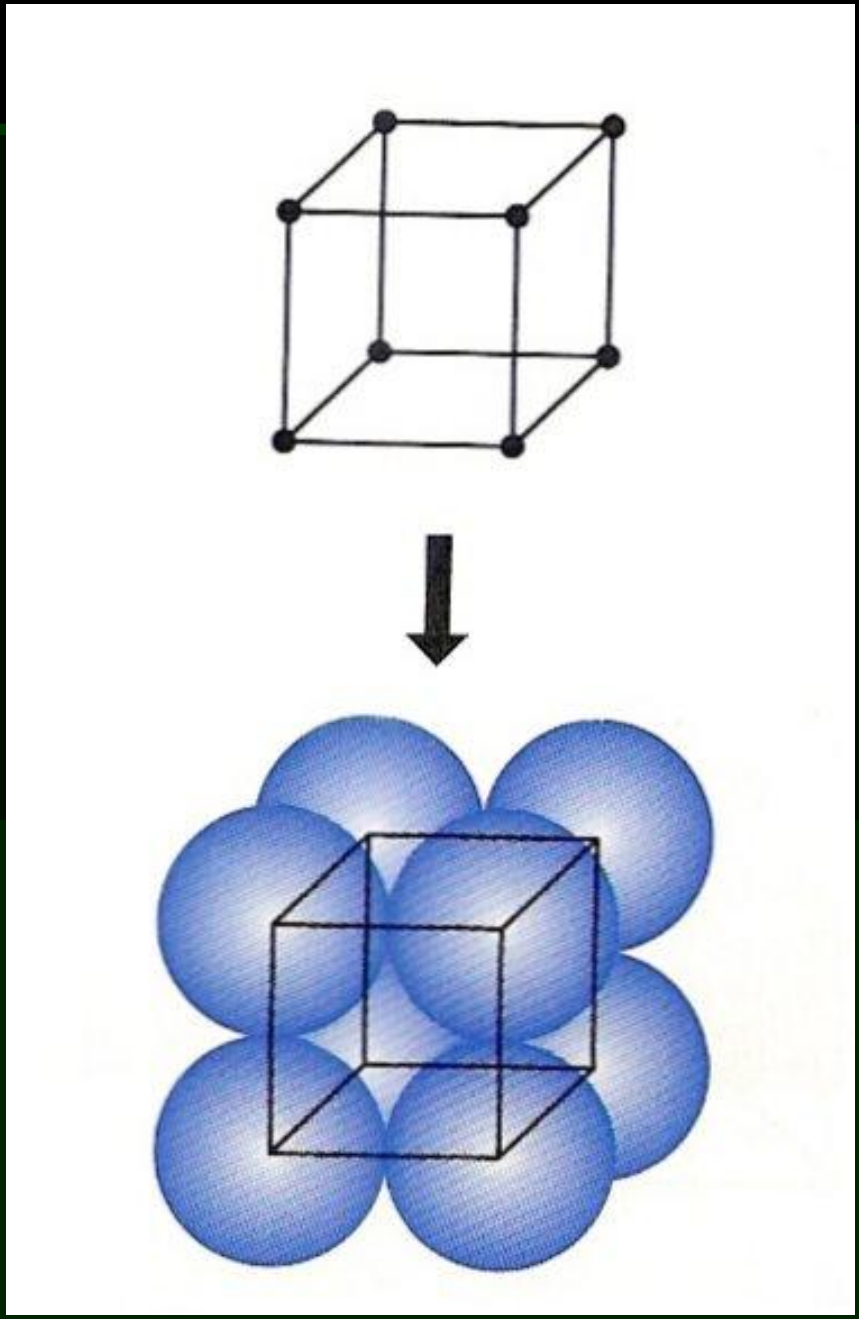
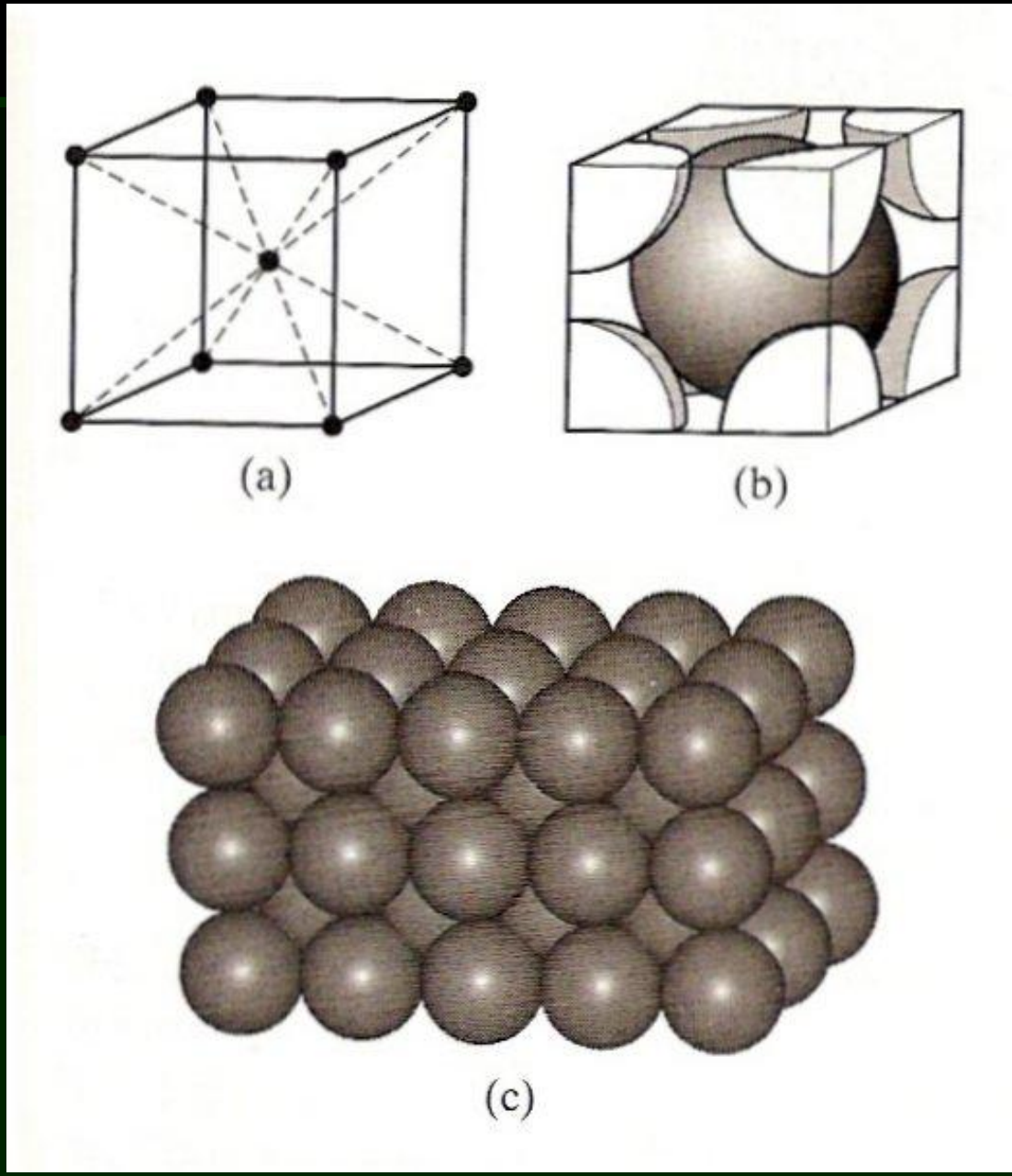
(Primitive) Cubic

- 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
  - α: 90.000°
  - β: 90.000°
  - γ: 90.000°



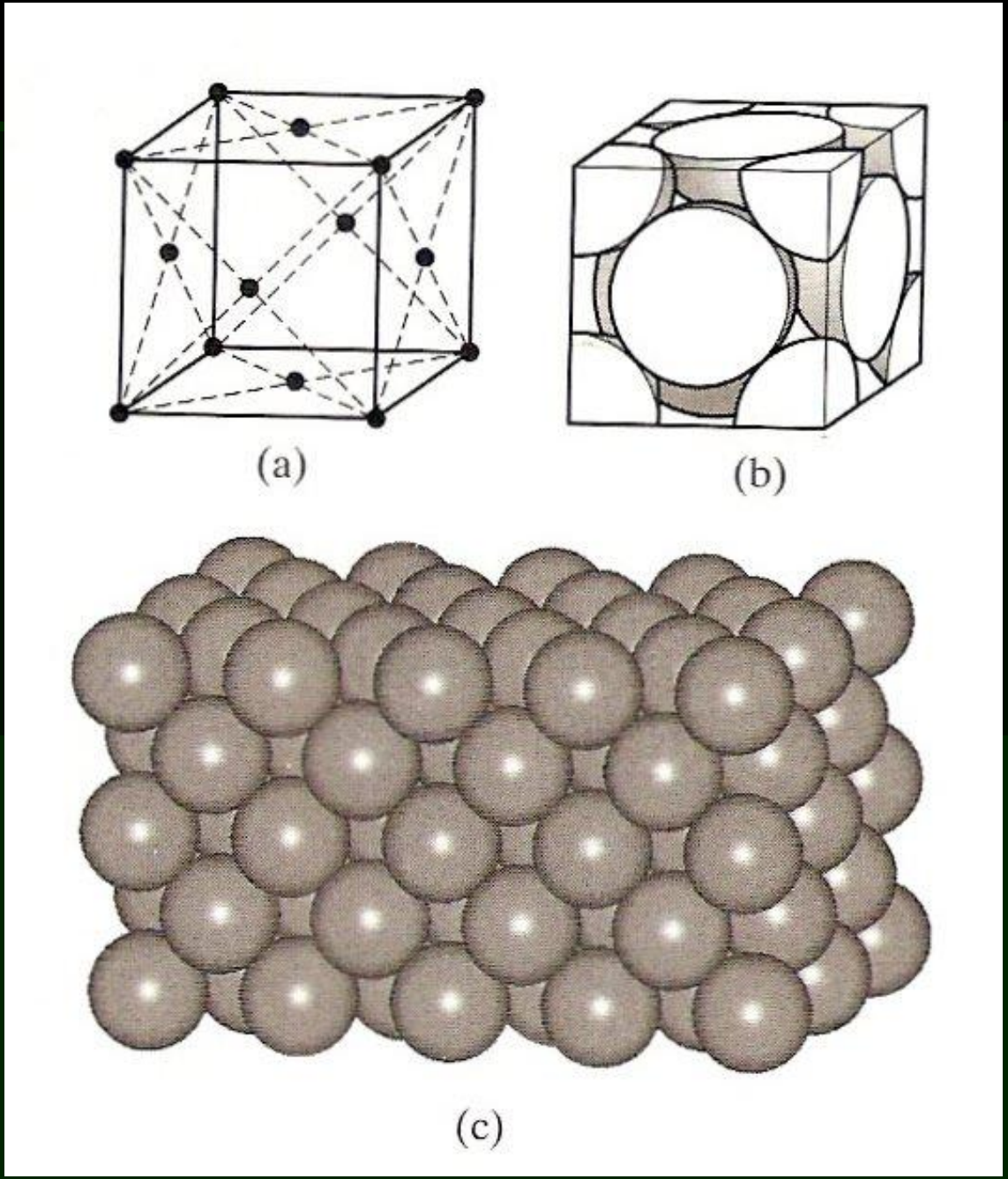
Body Centred Cubic (BCC)

- e.g. α-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
  - α: 90.000°
  - β: 90.000°
  - γ: 90.000°



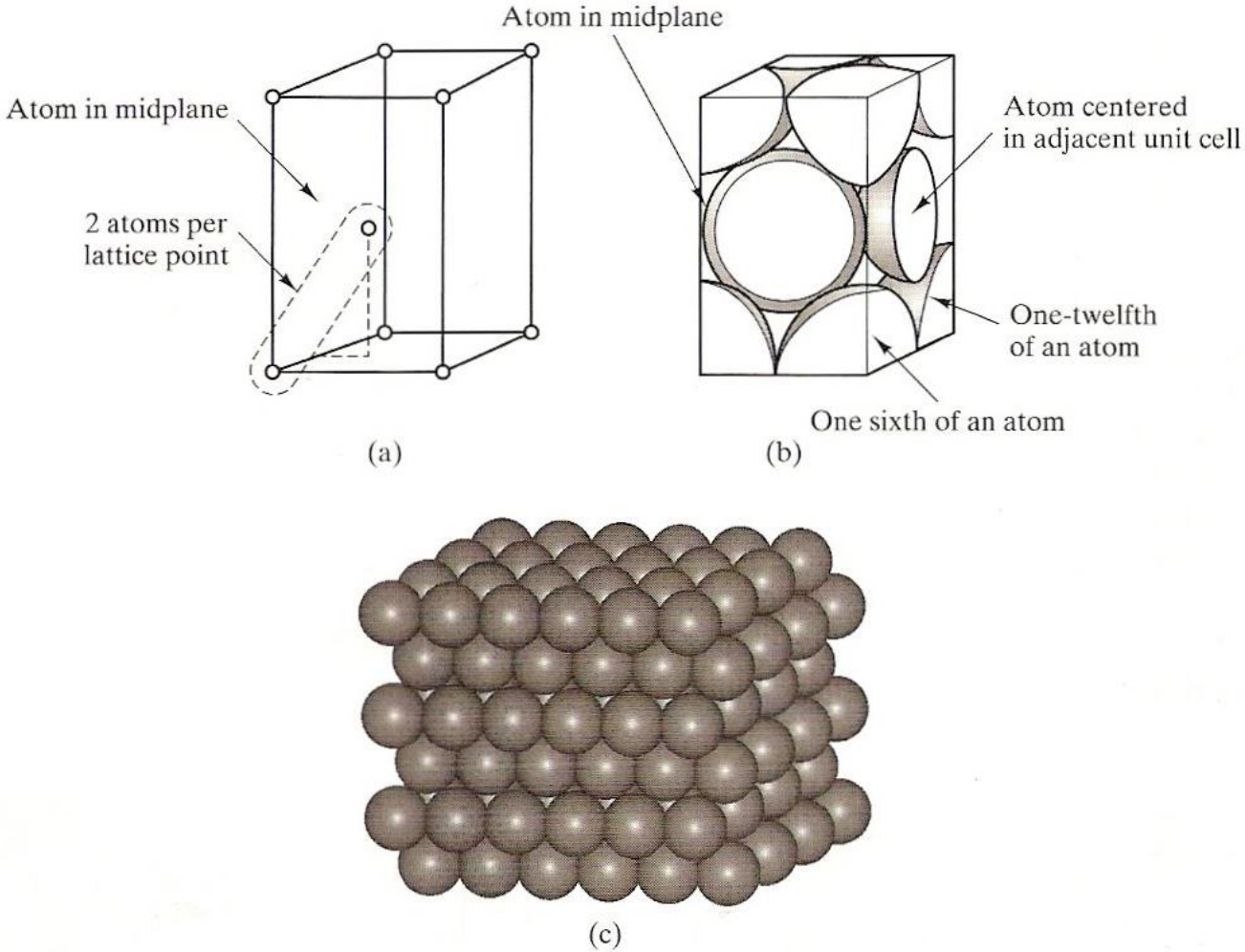
Face Centred Cubic (FCC)

- e.g. γ-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
  - α: 90.000°
  - β: 90.000°
  - γ: 90.000°

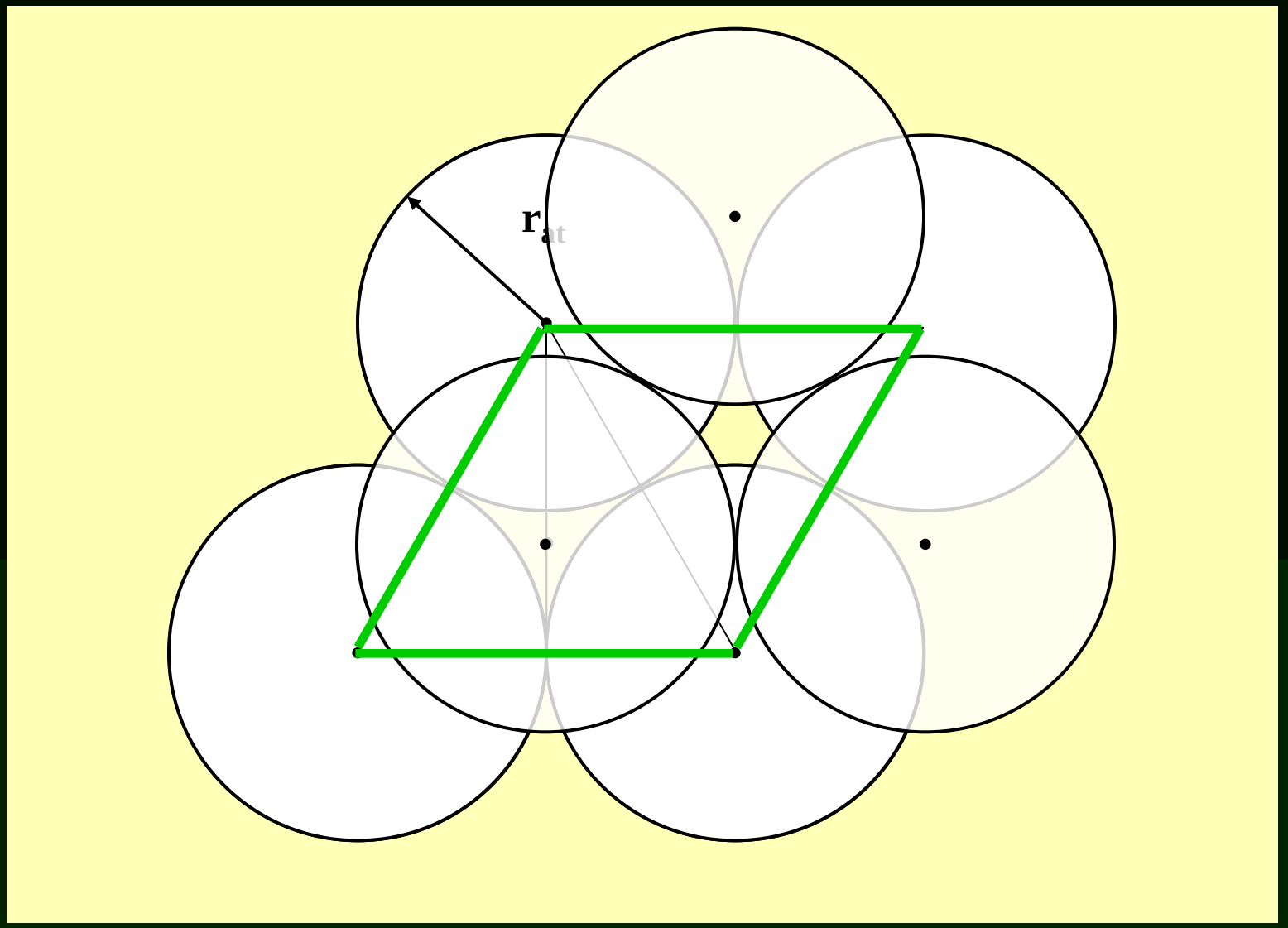


Hexagonal Close Packed (HCP)

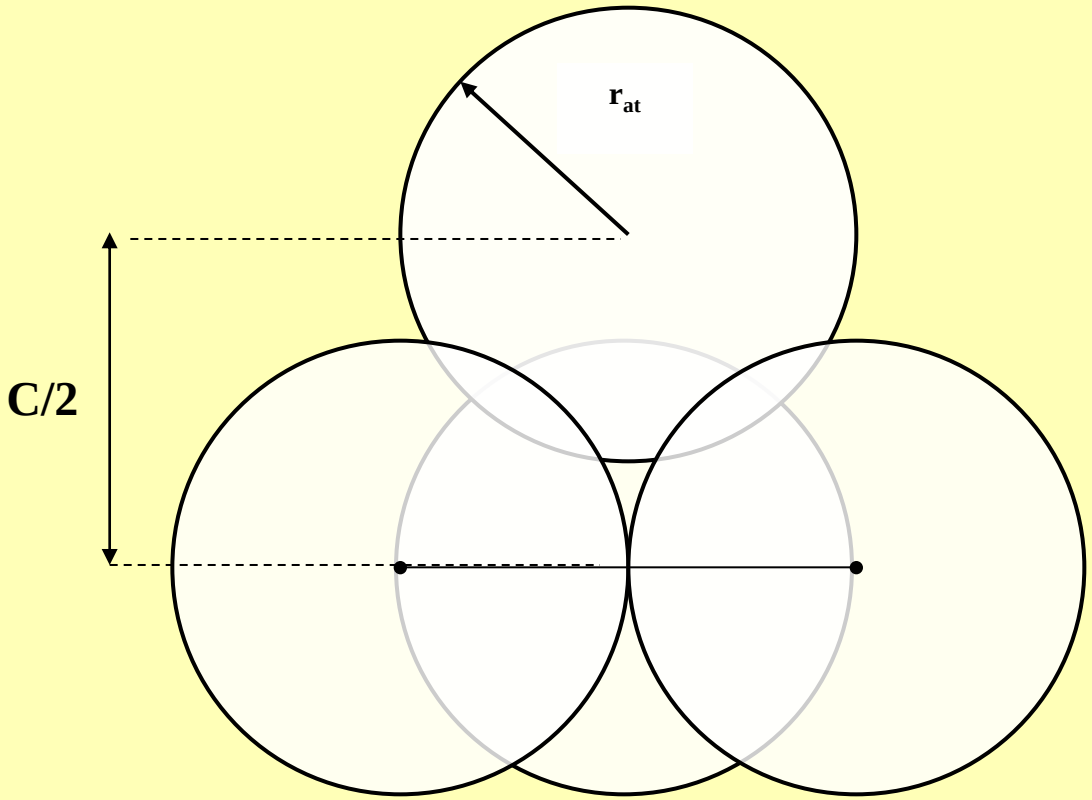
- e.g. Be, Mg, α-Ti, Zn, Zr
- Space group: P63/mmc
- (SG number: 194)
- **Zn** Structure: hcp
- Cell parameters:
  - *a*: 266.49 pm
  - *b*: 266.49 pm
  - *c*: 494.68 pm
  - α: 90.000°
  - β: 90.000°
  - γ: 120.000°



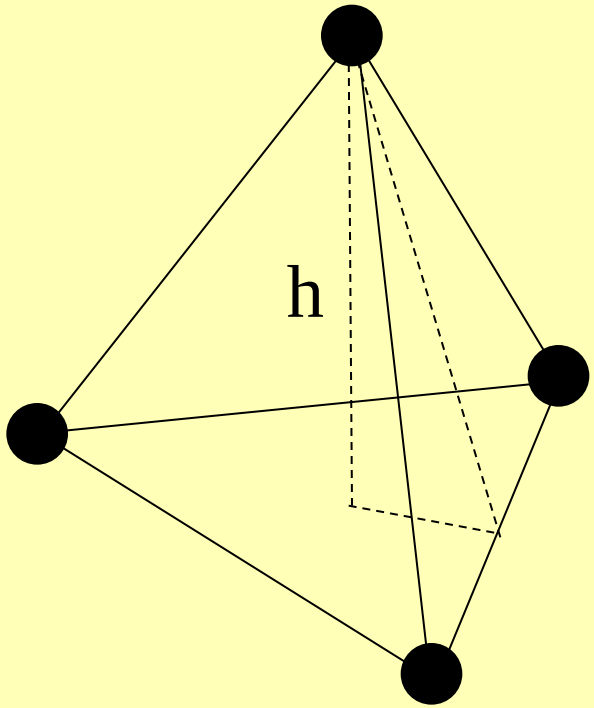
HCP Unit cell – plan view



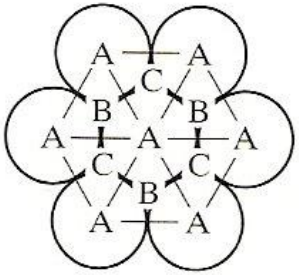
HCP Unit cell – side view



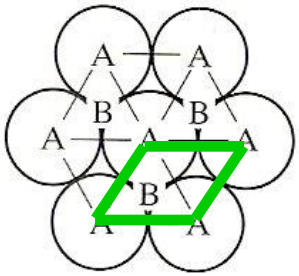
HCP reduced sphere view



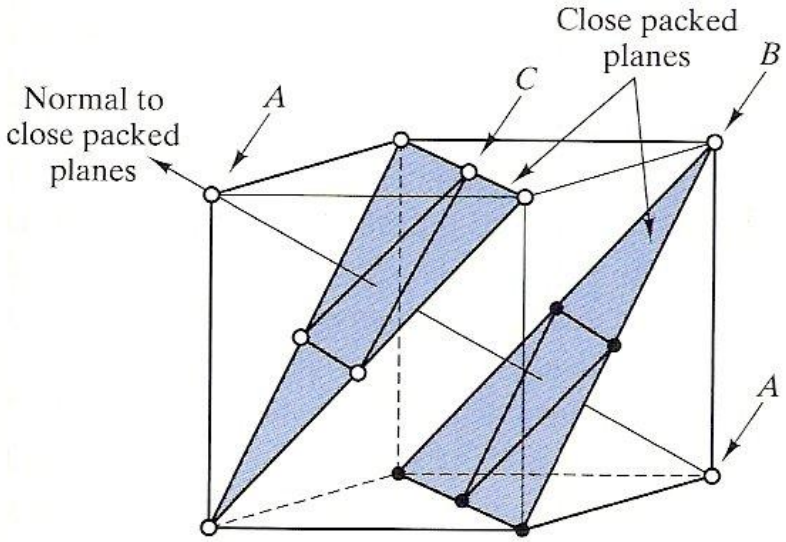
Close Packing FCC vs. HCP



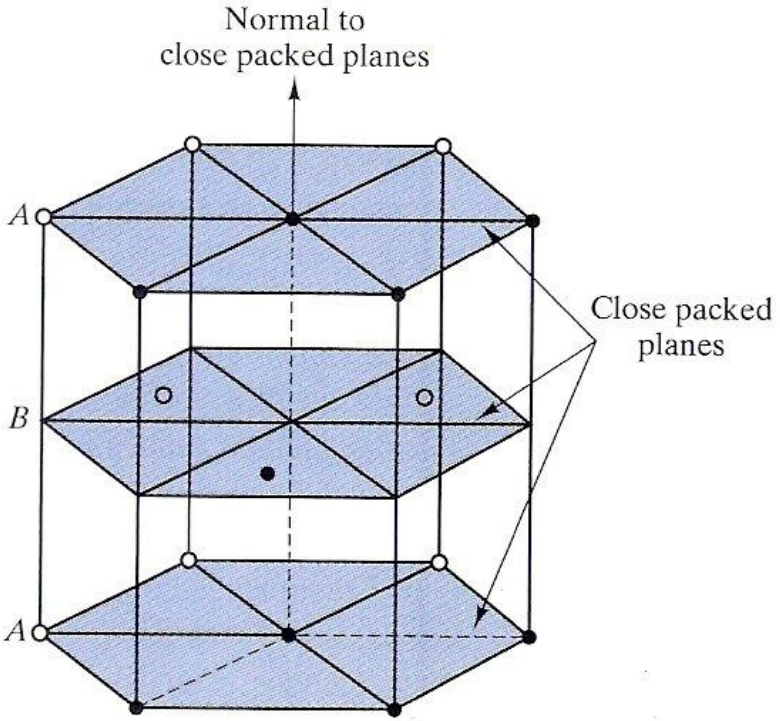
(a) Stacking of close packed planes



(b) Stacking of close packed planes



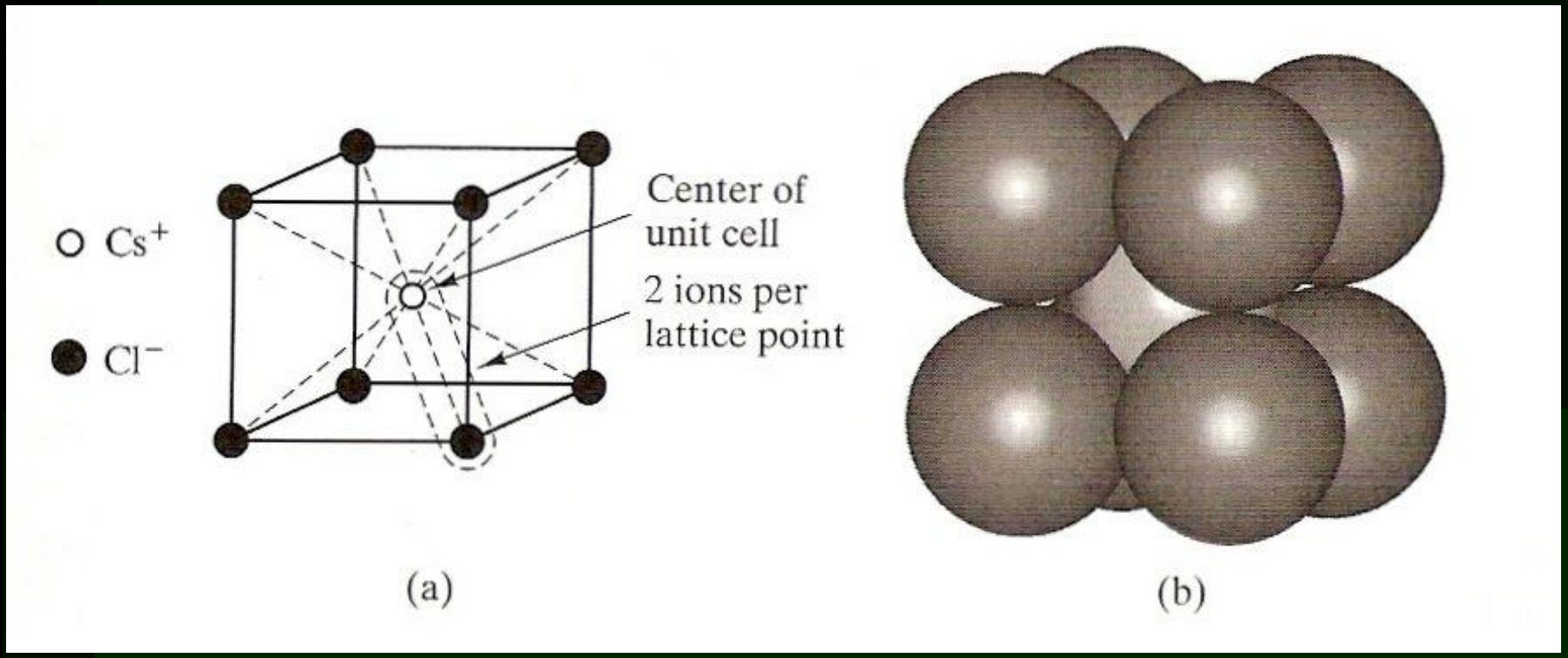
(c) Face-centered cubic



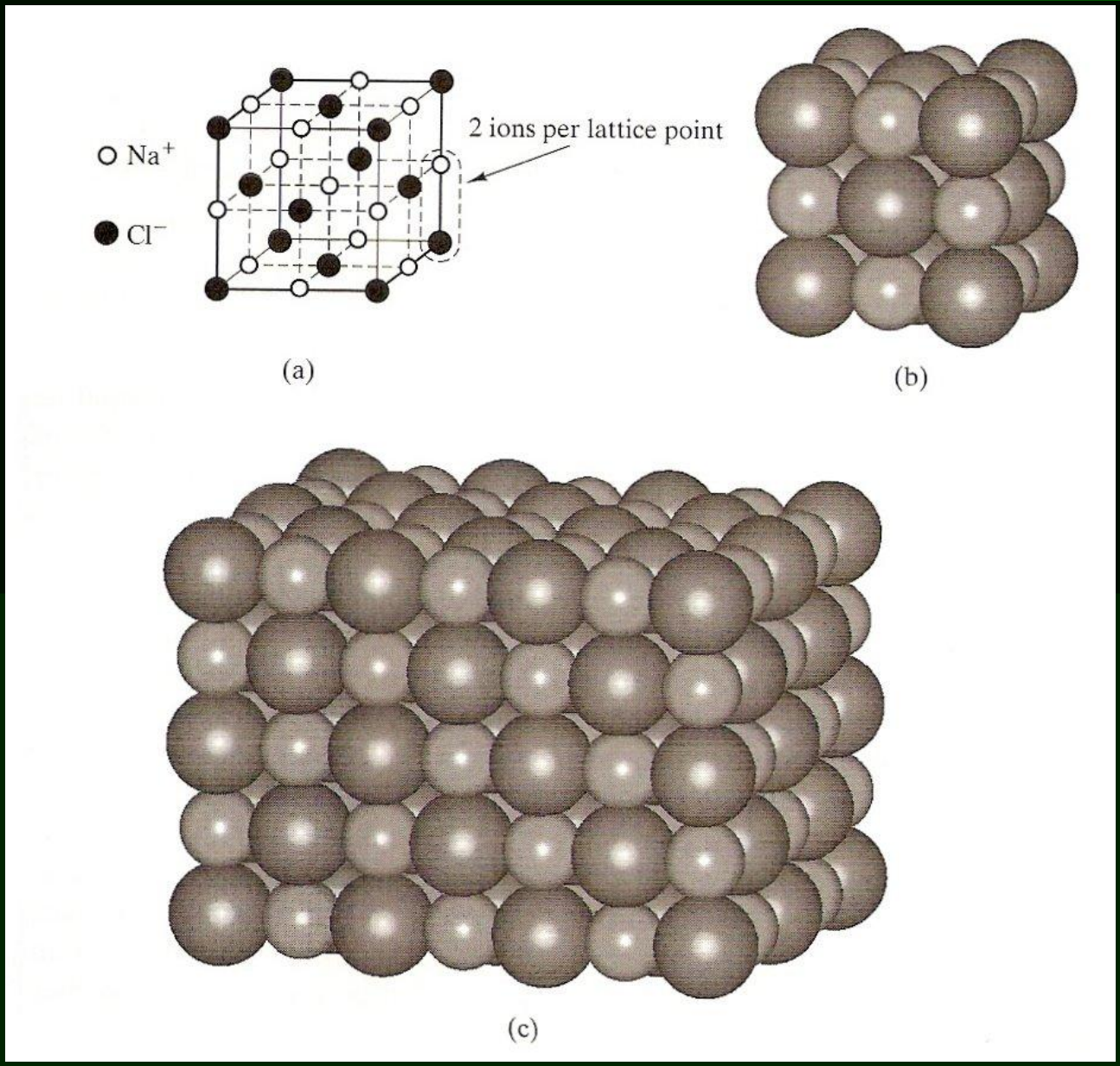
(d) Hexagonal close packed

Caesium chloride Cubic

- (Primitive) cubic

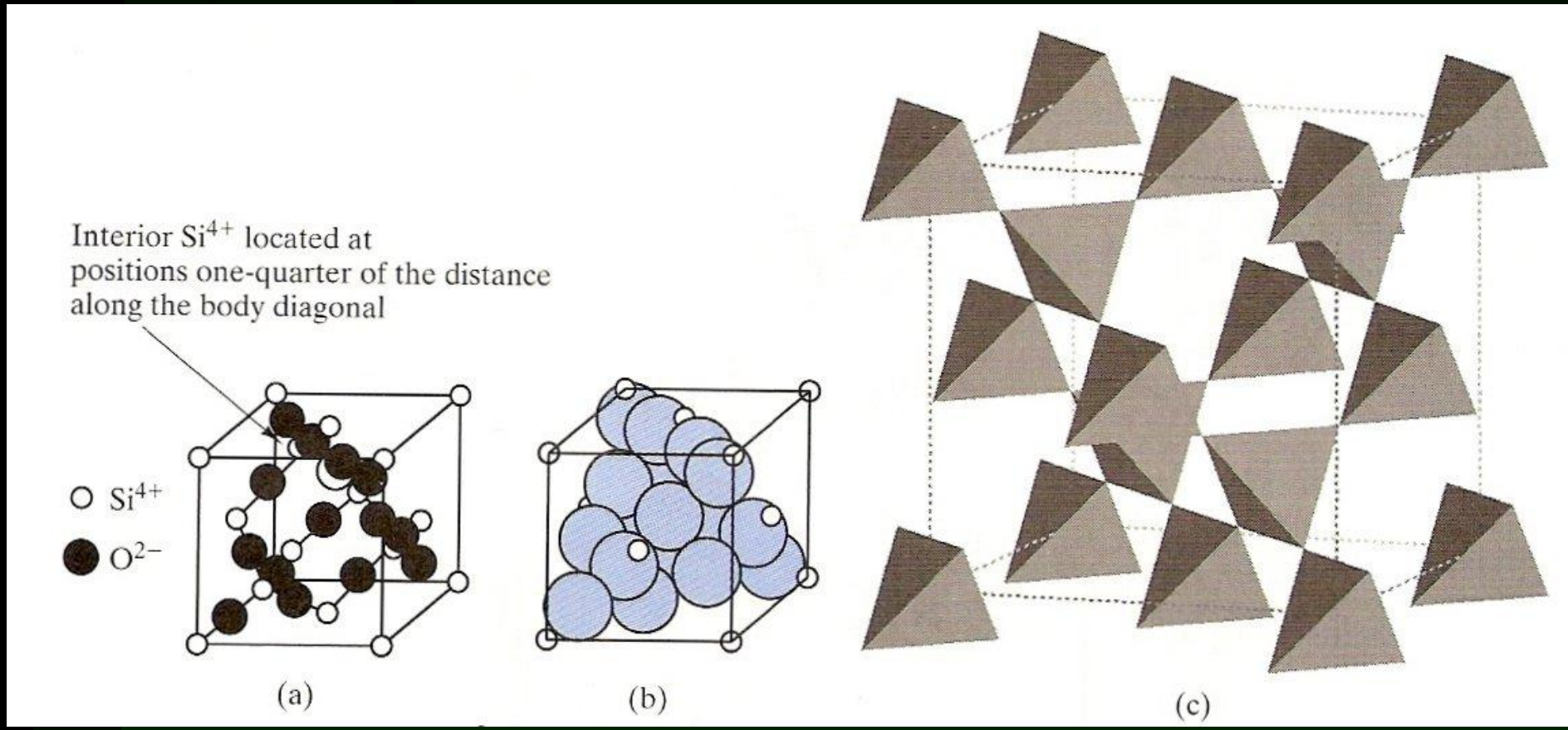


Sodium chloride FCC



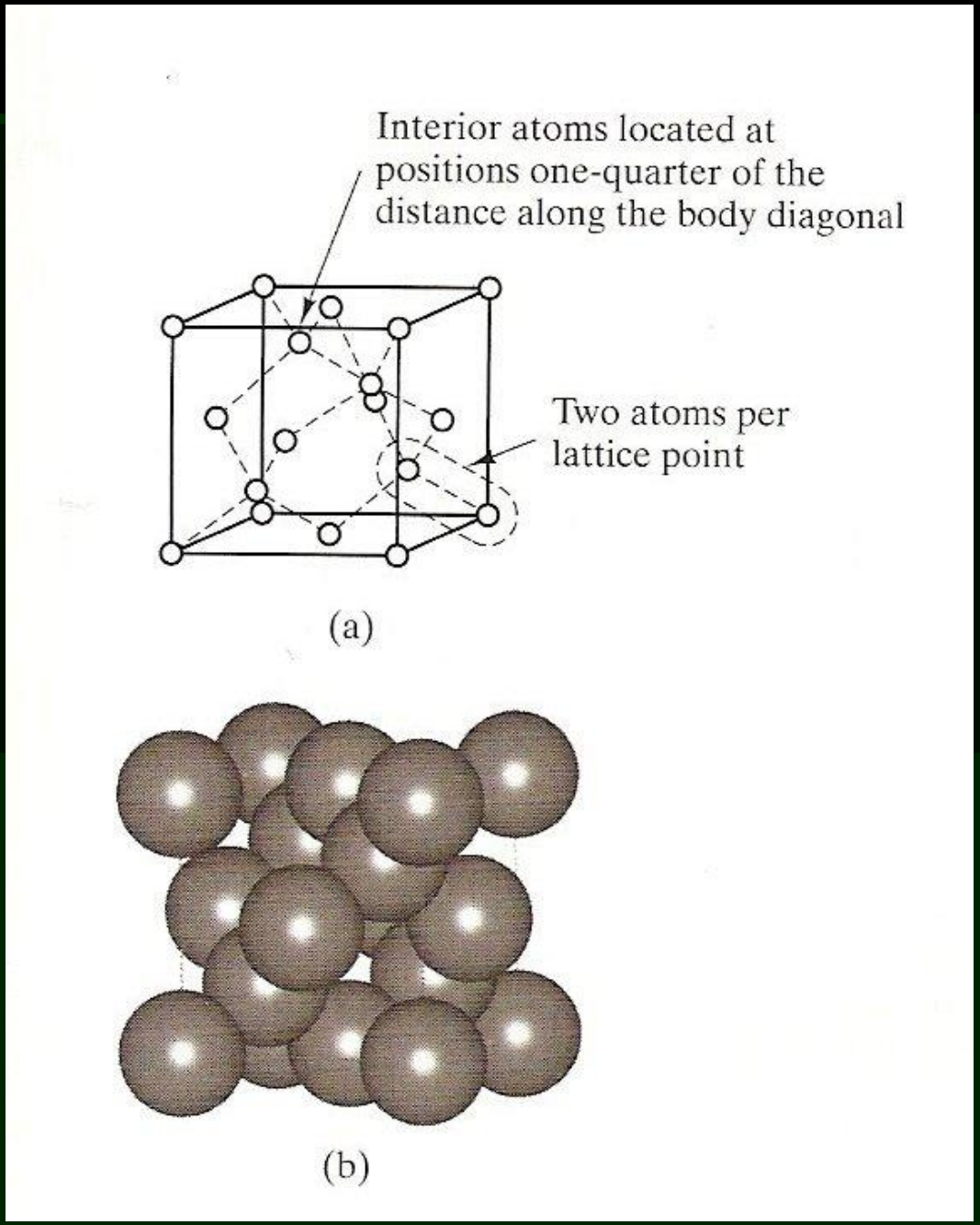
Cristobalite FCC

- e.g. SiO_2



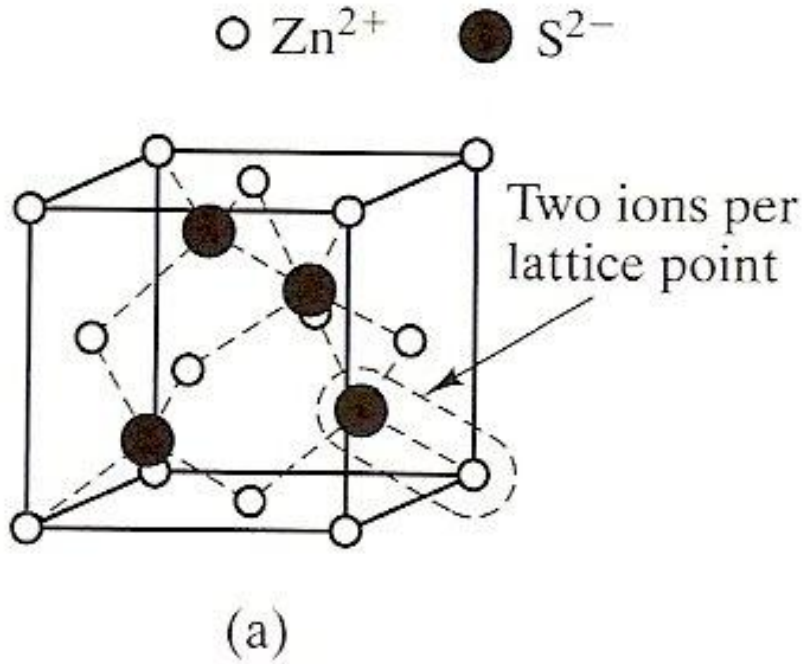
Diamond cubic (FCC)

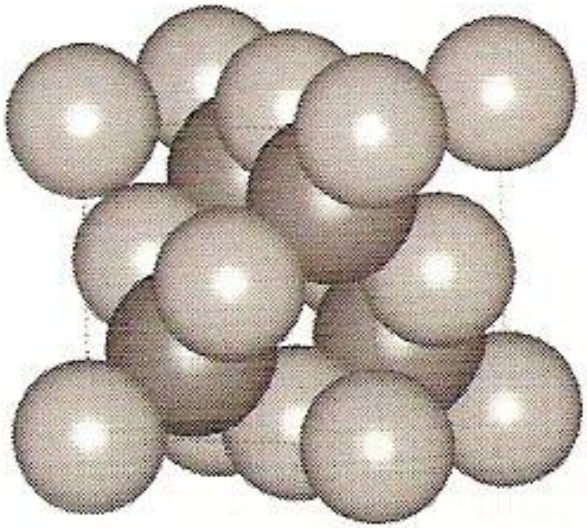
- e.g. Si, Ge, grey-Sn



Zinc blende (FCC)

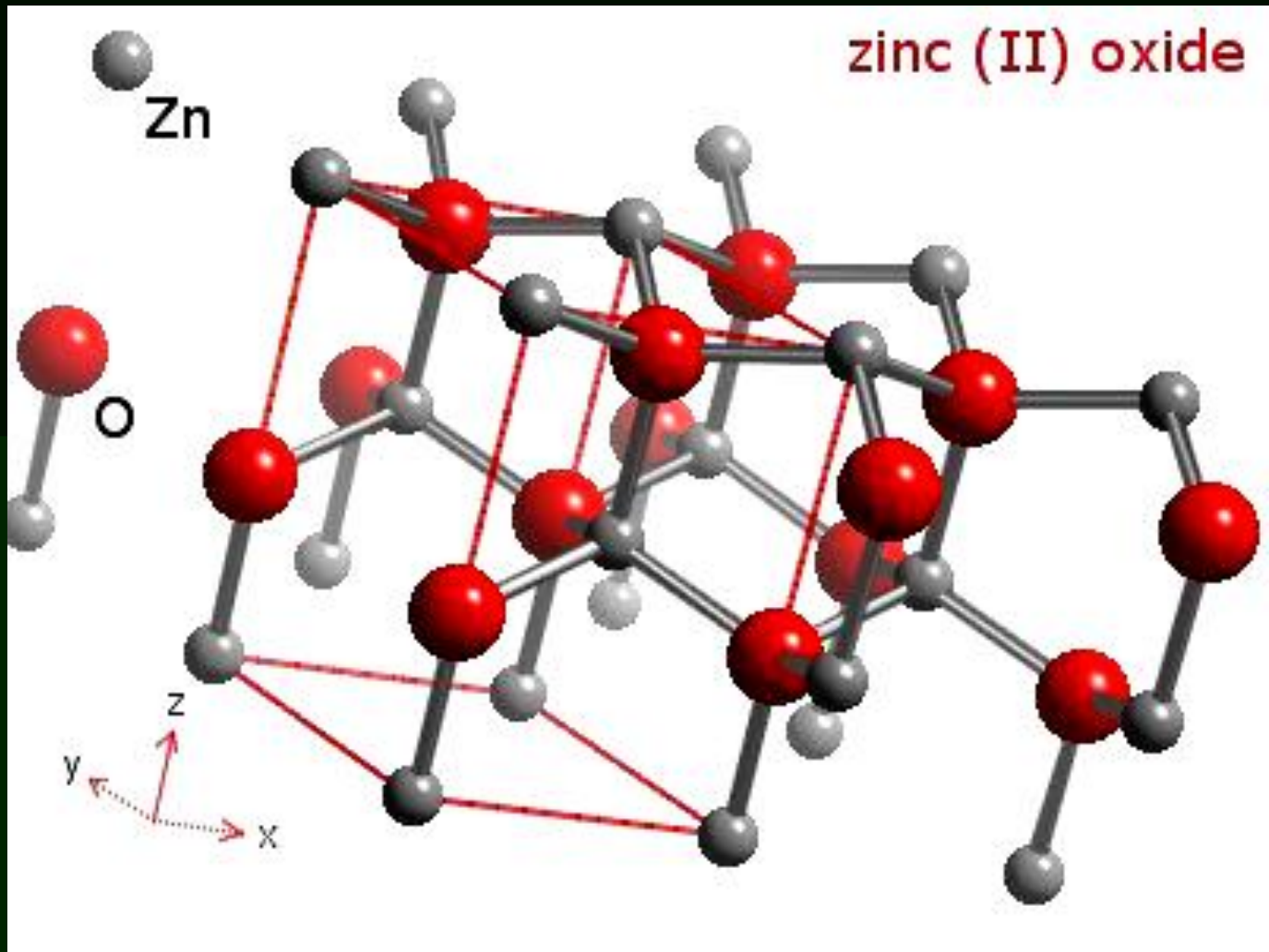
- e.g. GaAs, AlP, InSb (III-V SCs) ZnS, CdS, HgTe (II-VI SCs)





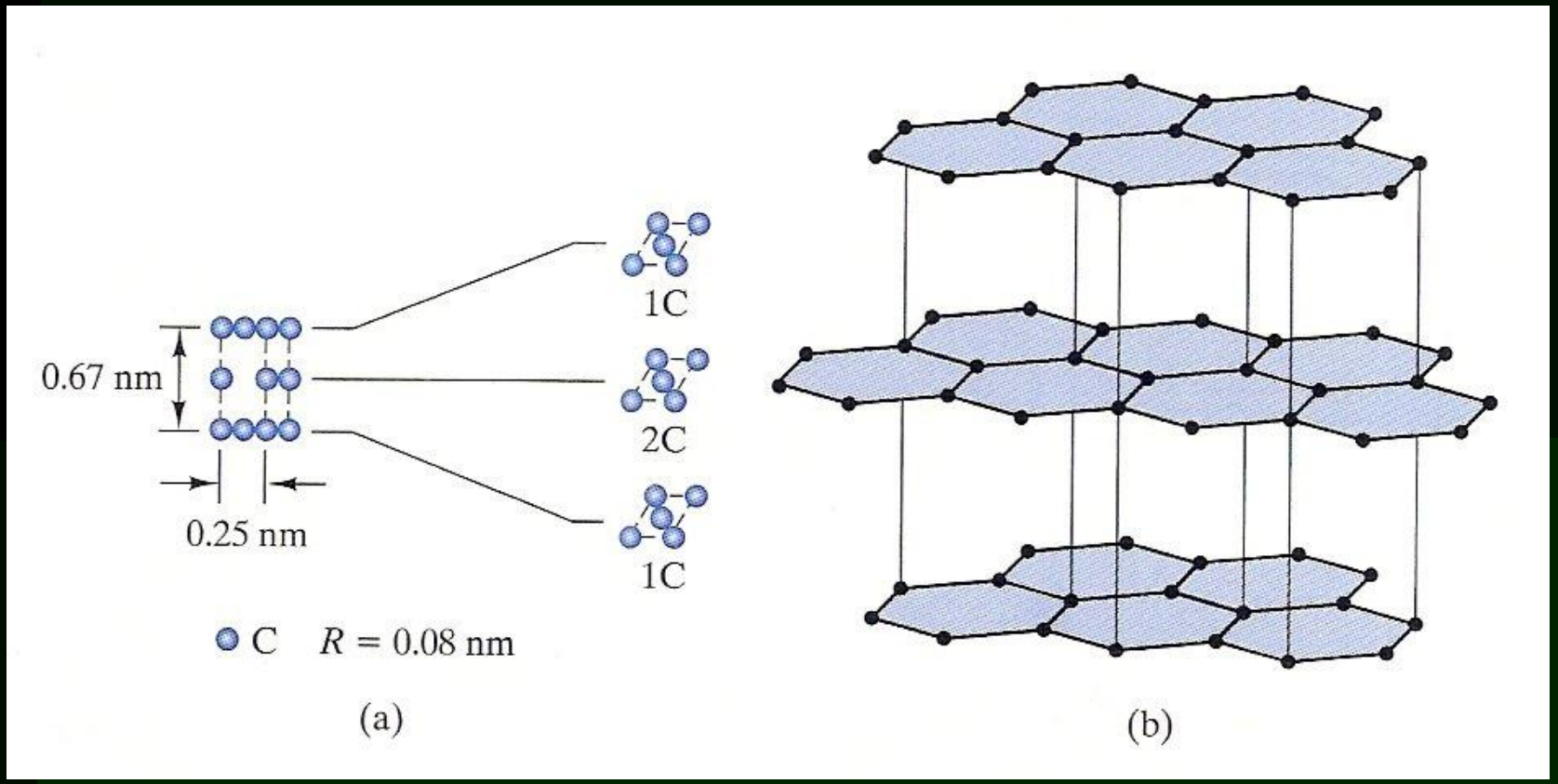
Wurtzite (Hexagonal)

- e.g. ZnS, ZnO, CdS



Carbon polymorphism

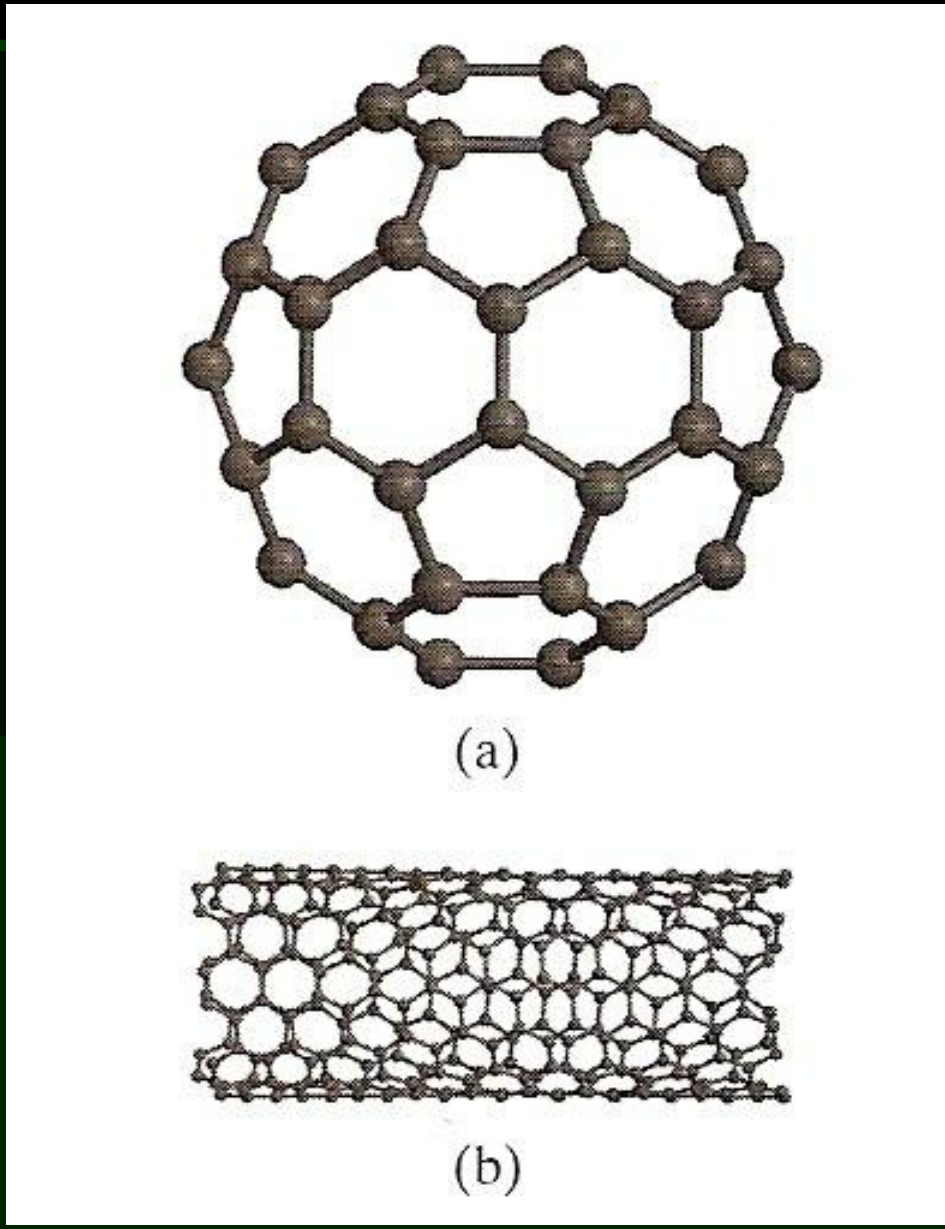
- Graphite



Carbon polymorphism

- Buckminster Fullerene C60

- Carbon nanotube



Caculation of Density

- The density of a crystaline material can be calculated by

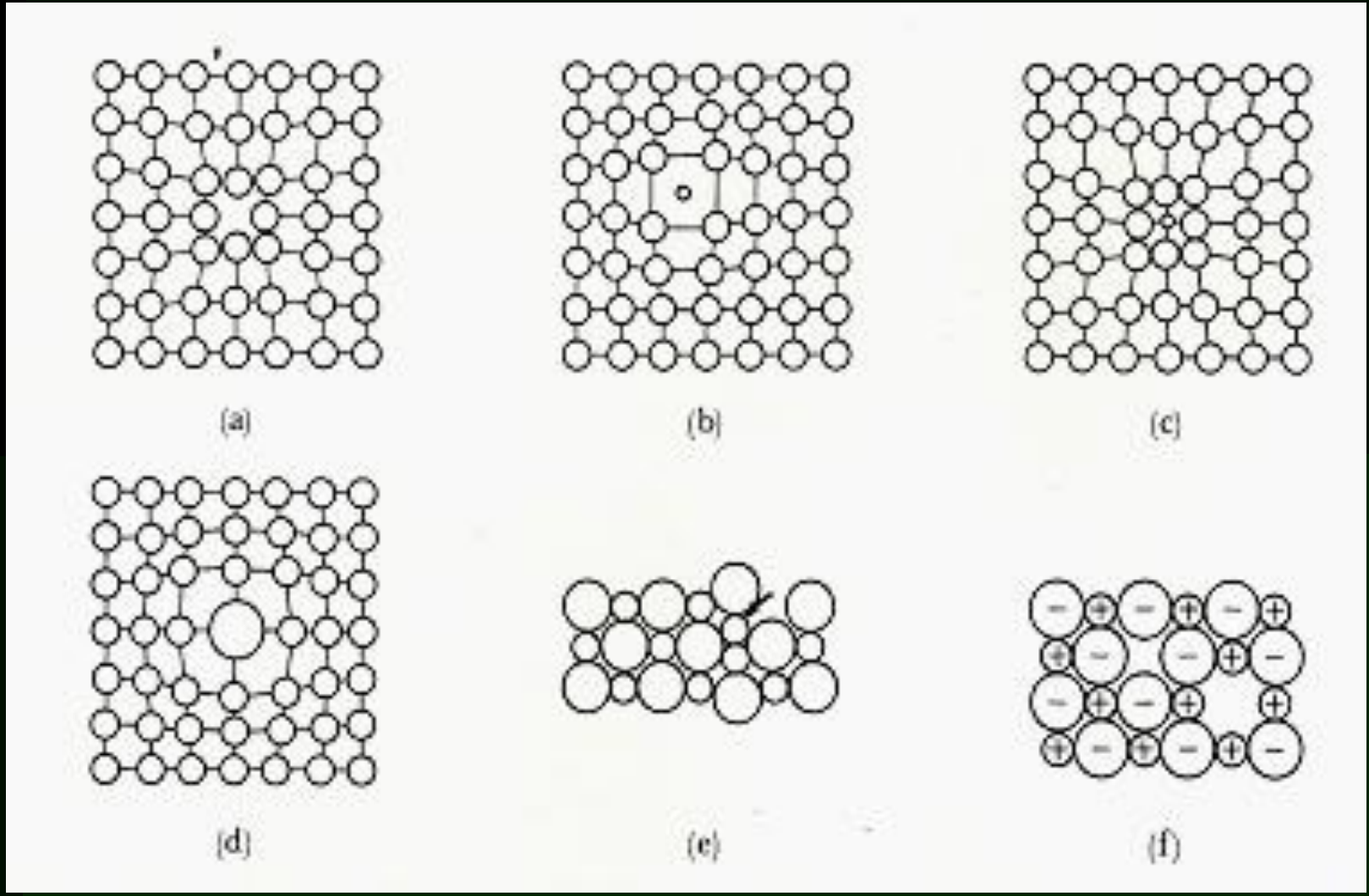
$$\rho = \frac{n\,.\,atomic\ mass}{Vol_{Unit\,Cell}}$$

or

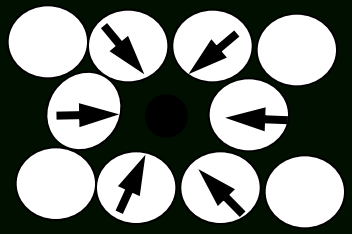
$$\rho = \frac{n\,.\,atomic\ weight}{N_A\ .Vol_{Unit\,Cell}}$$

Imperfections

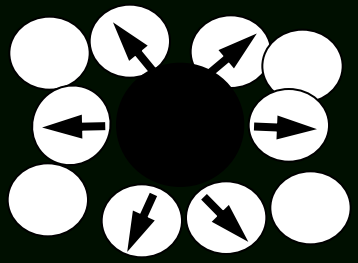
- Point defects



Lattice strains



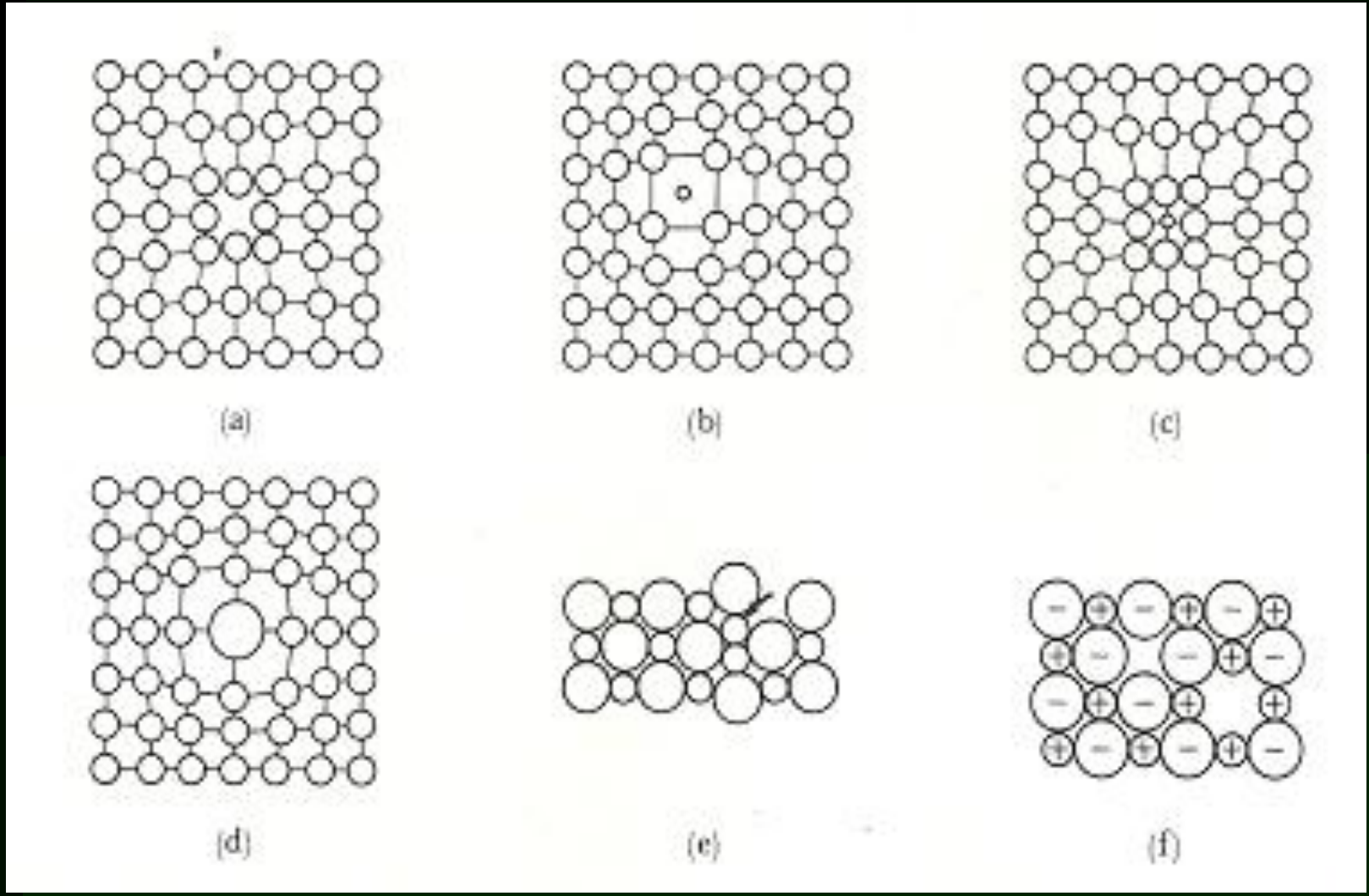
Tensile



Compressive

Notice lattice strains

- Point defects



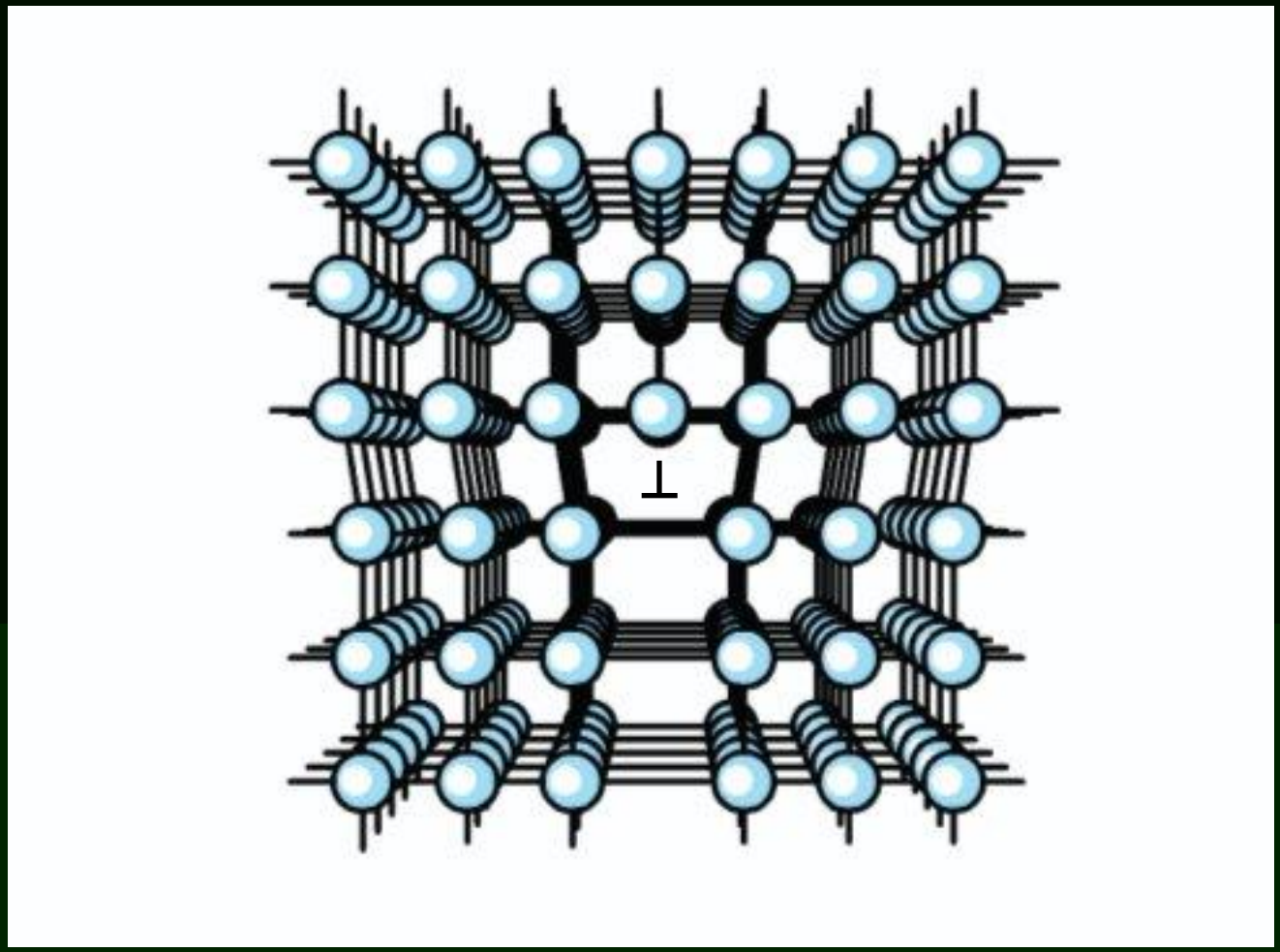
Number of Defects

- Number of vacancies (N_V) is given by

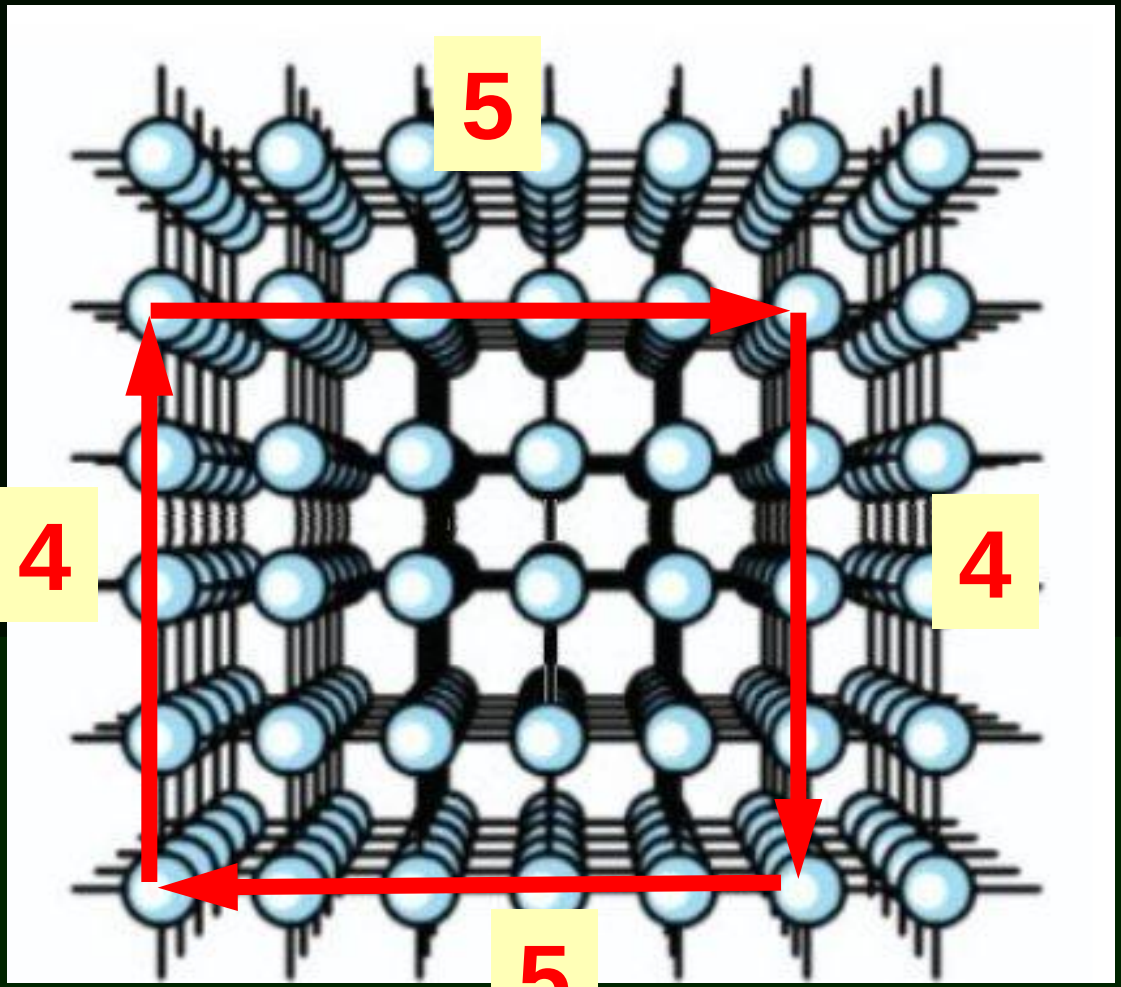
$$N_V = N_0 e^{-E_a / kT}$$

where N_0 is number of atomic sites and E_a is the activation energy for the formation of a vacancy.

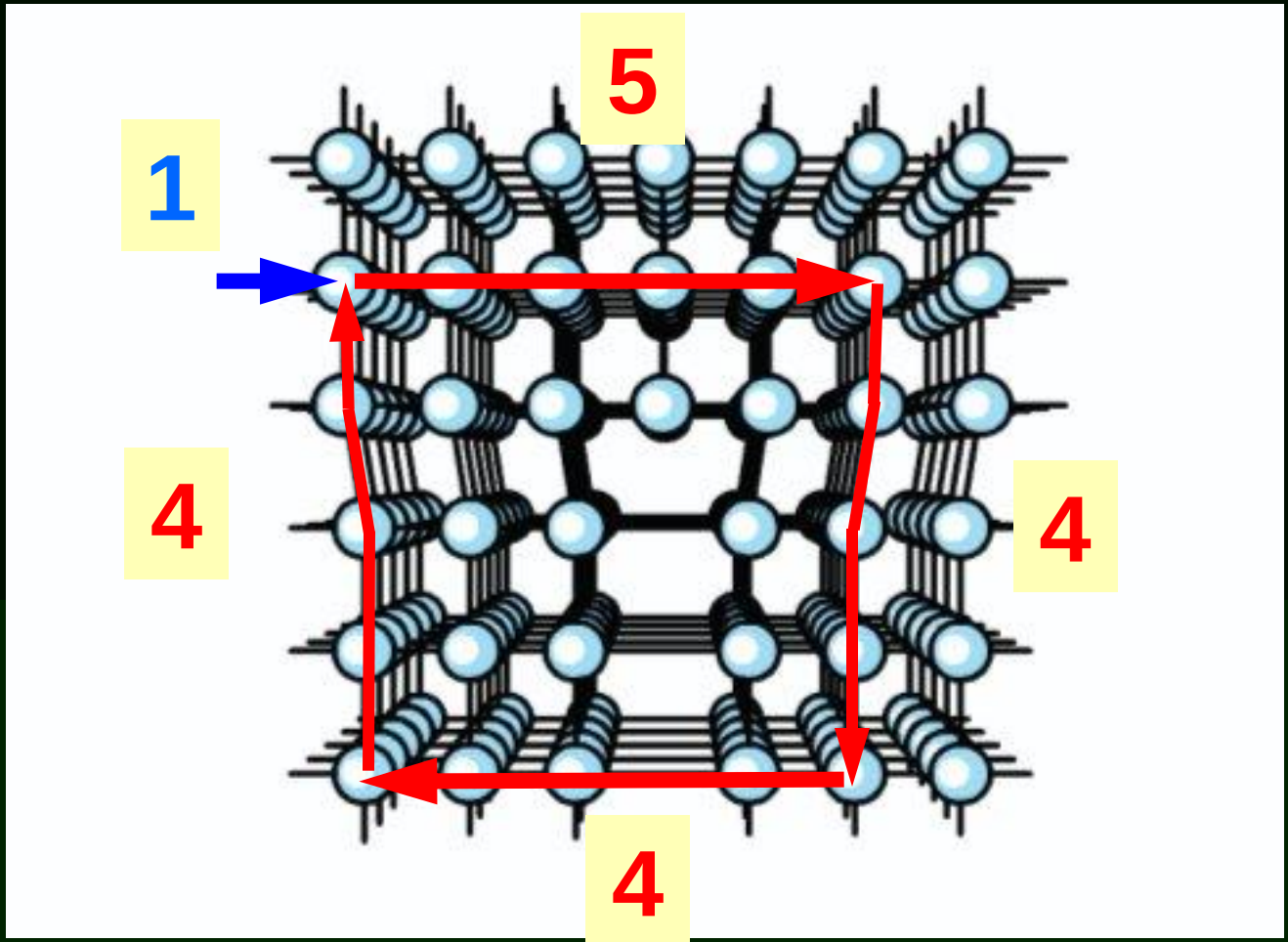
Edge Dislocation



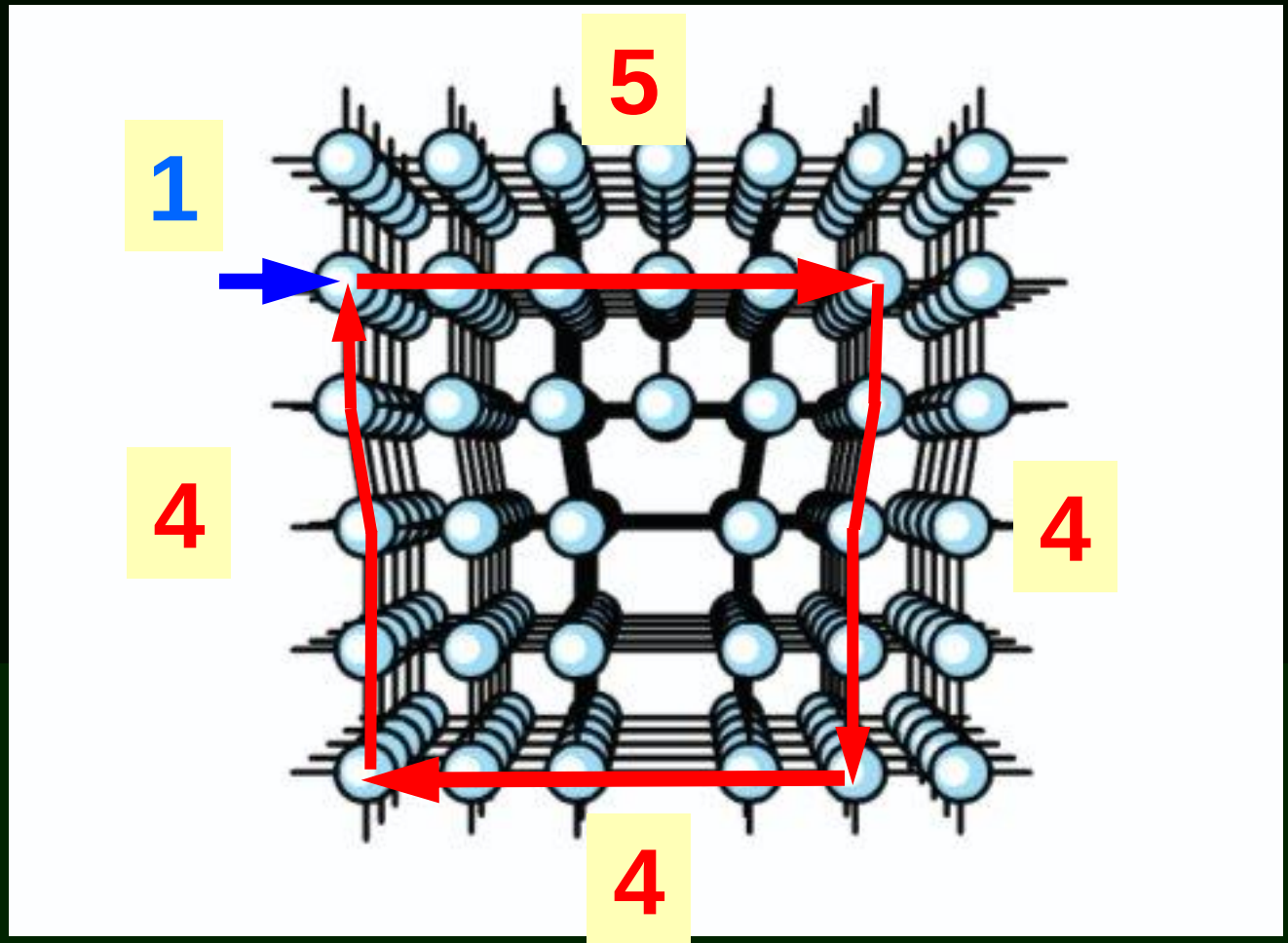
Perfect Crystal



Edge Dislocation

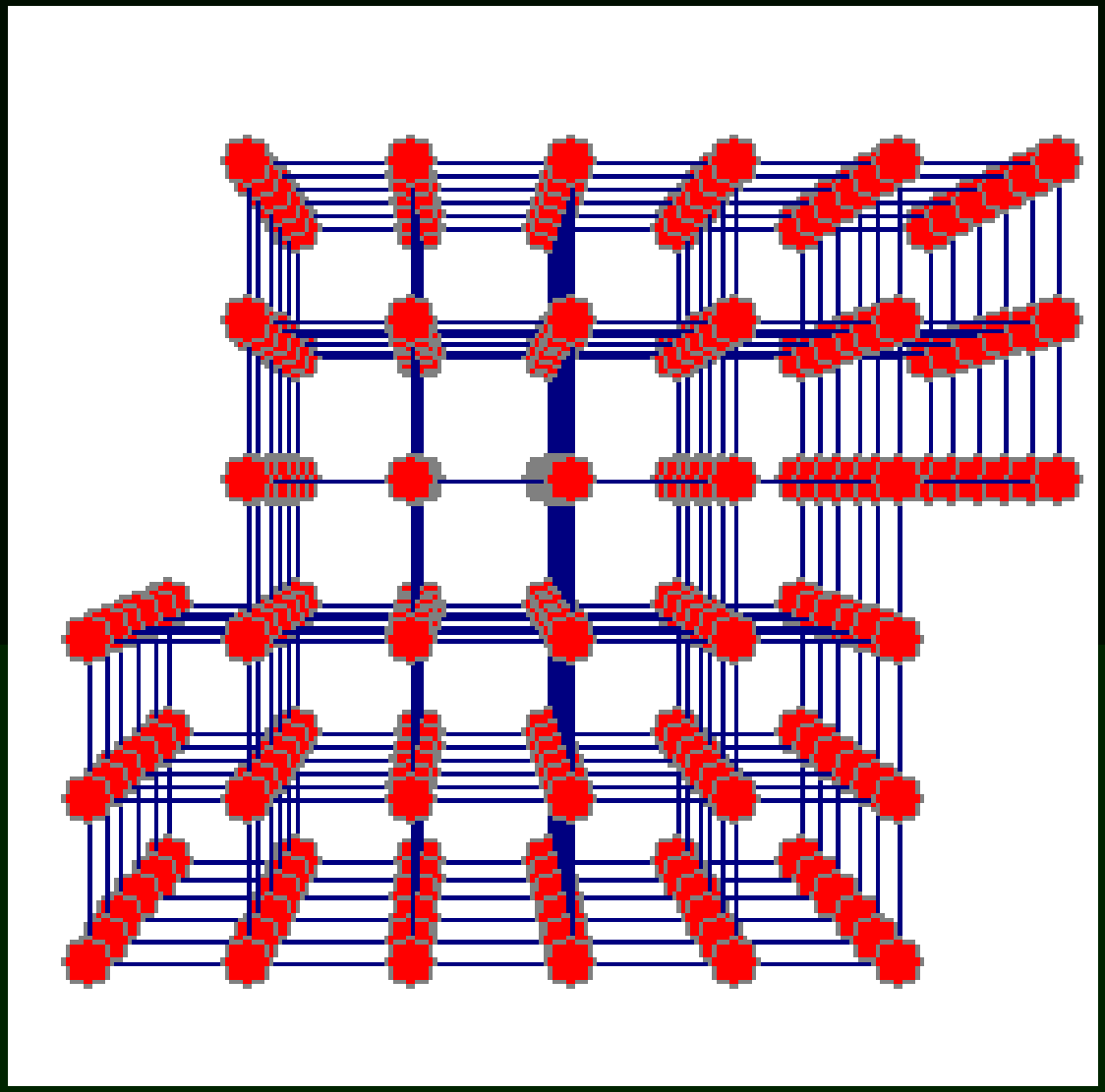


Burgers Vector

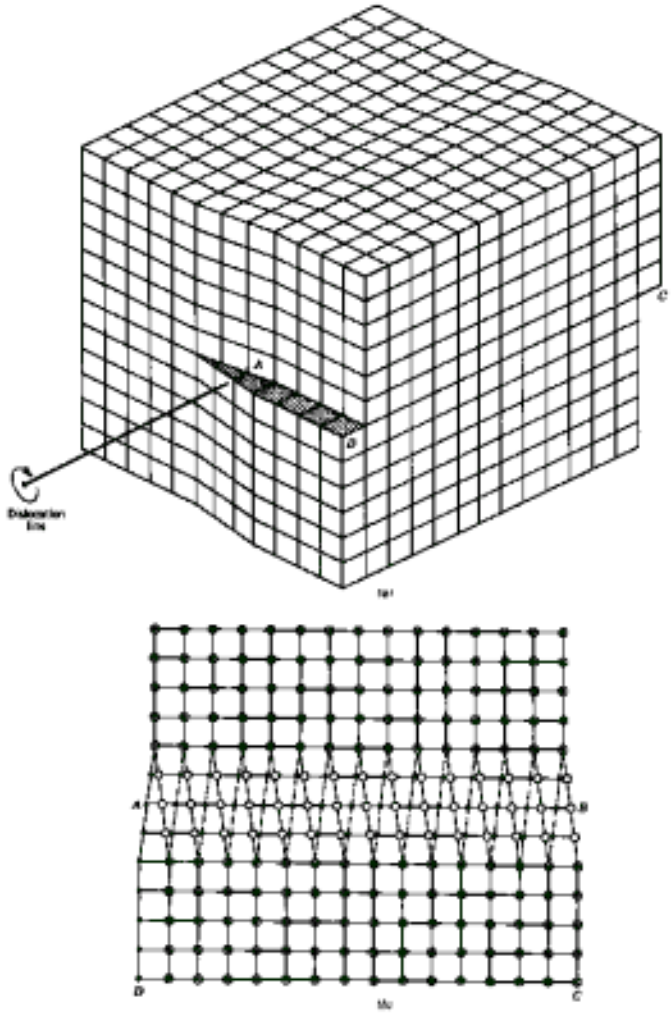


- The vector necessary to complete ‘close’ a path ‘surrounding’ the dislocation.

Edge Dislocation Motion



Screw Dislocation



Screw Dislocation

Screw Dislocation viewed from above

Dislocation along line AB

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

William D. Callister, Jr. Materials Science and Engineering, An Introduction. John Wiley & Sons, Inc. 1985