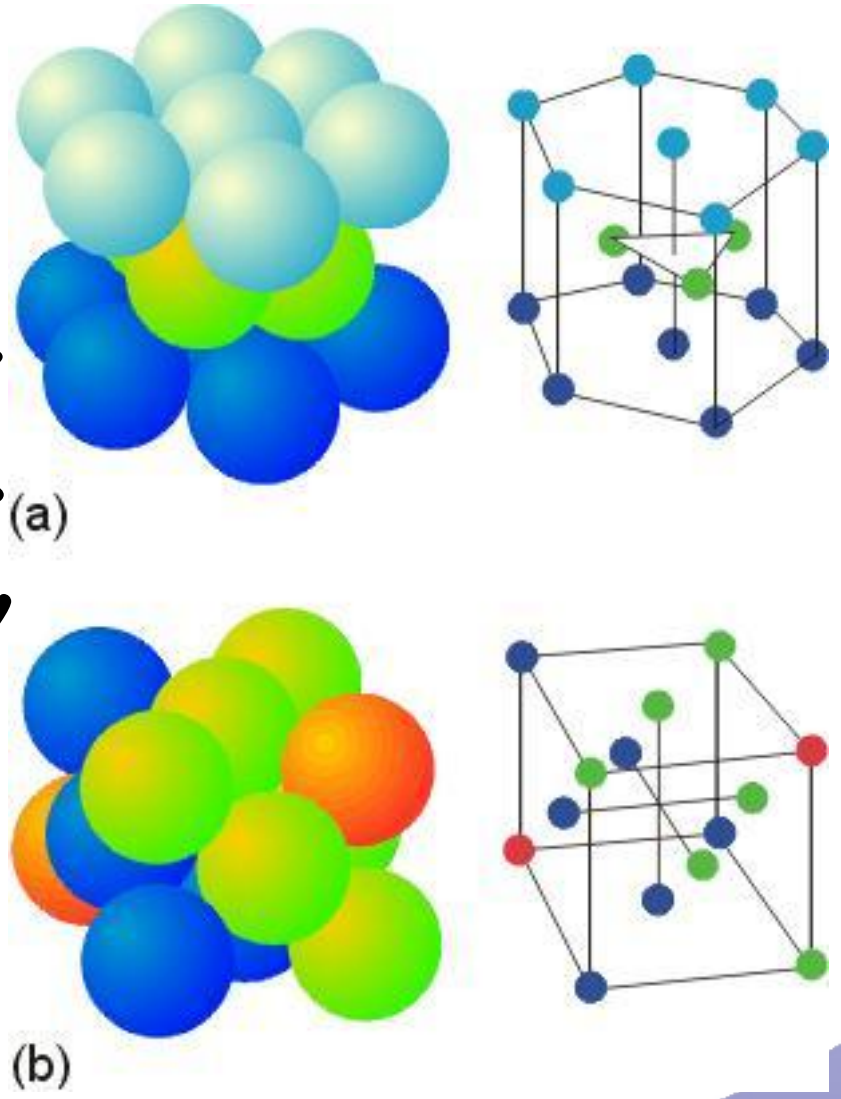
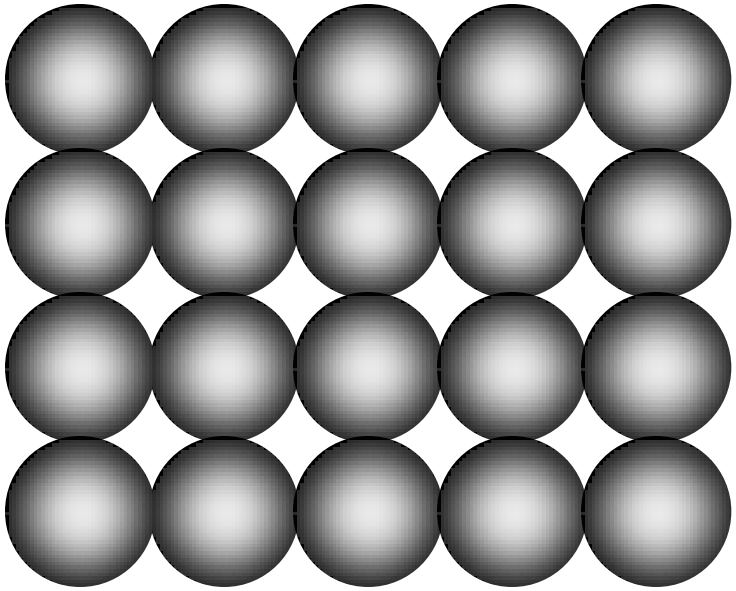
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

CLOSE PACKING GEOMETRY



pranjoto utomo

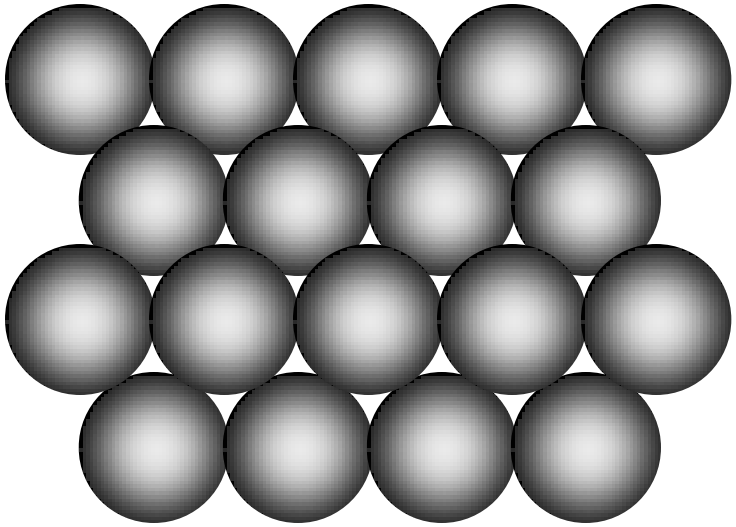
Packing types



SIDE BY SIDE

PACKING

NOT A CLOSEST PACKING



HEXAGONAL

PACKING

CLOSEST PACKING

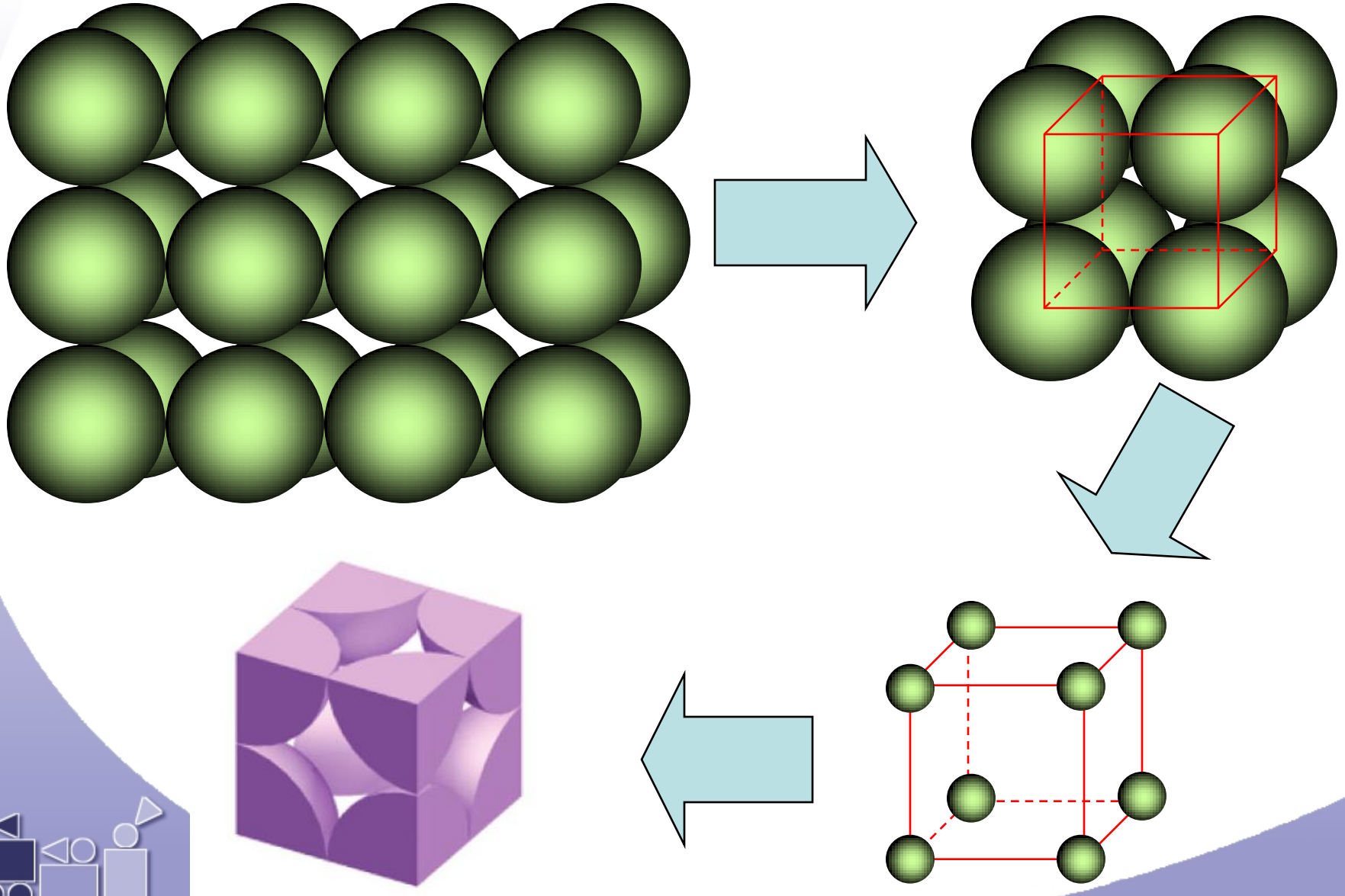
Side-by-side packing

Expanding of side-by-side packing types

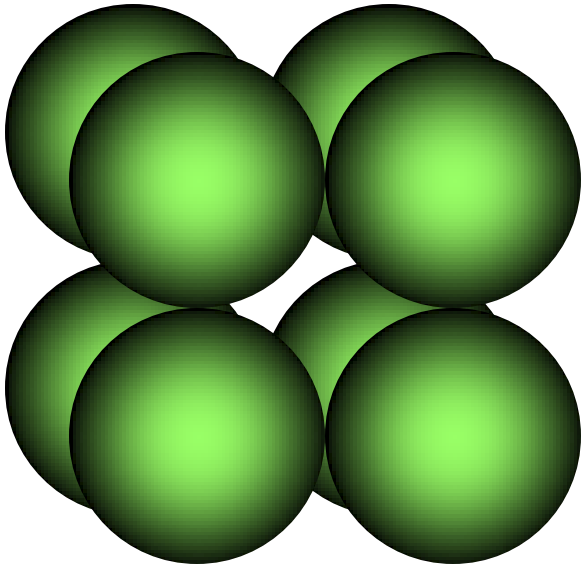
1. SIMPLE (PRIMITIVE) CUBIC (SC)

1. BODY CENTERED CUBIC (BCC)

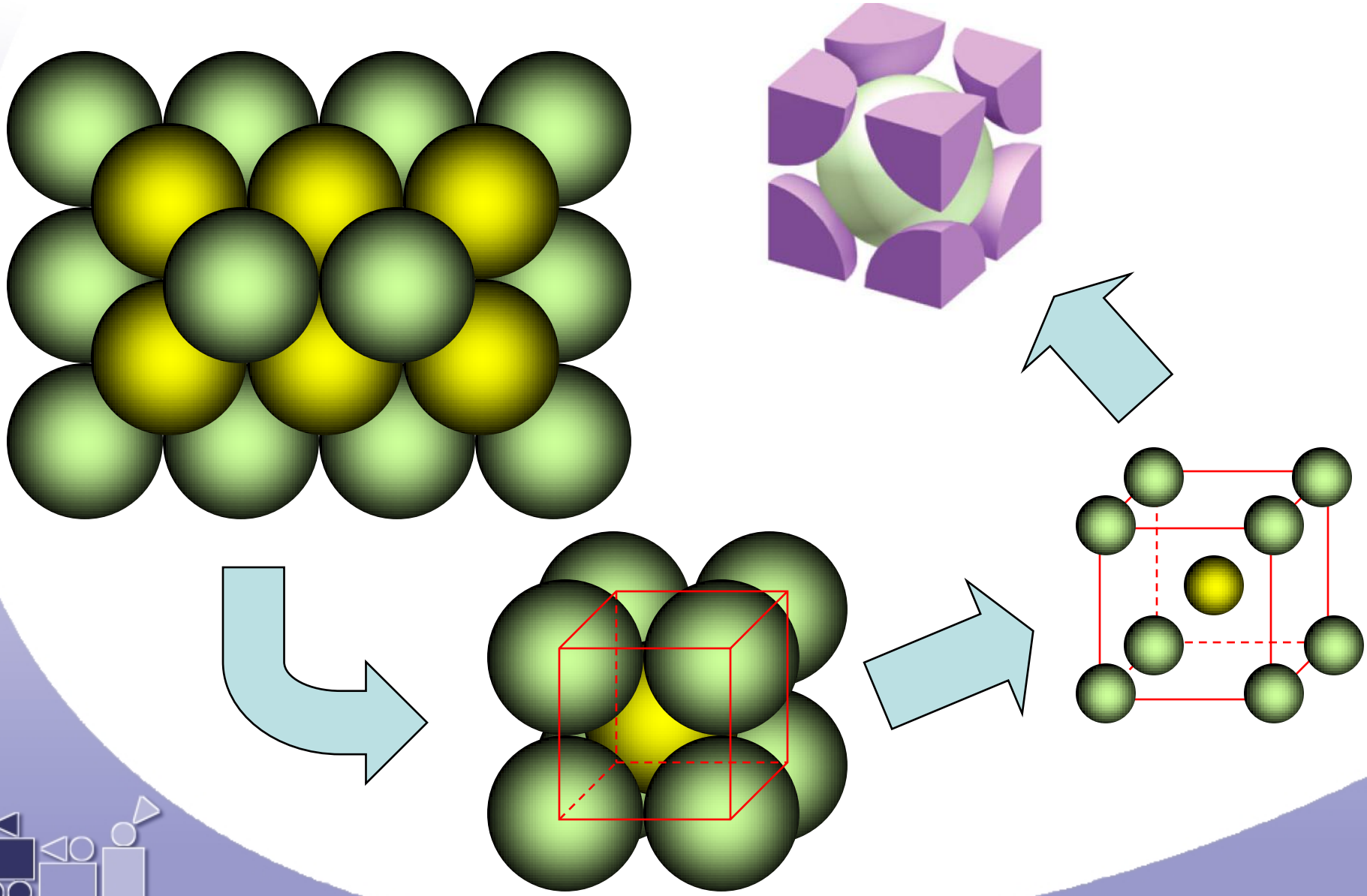
SIMPLE CUBIC (SC)



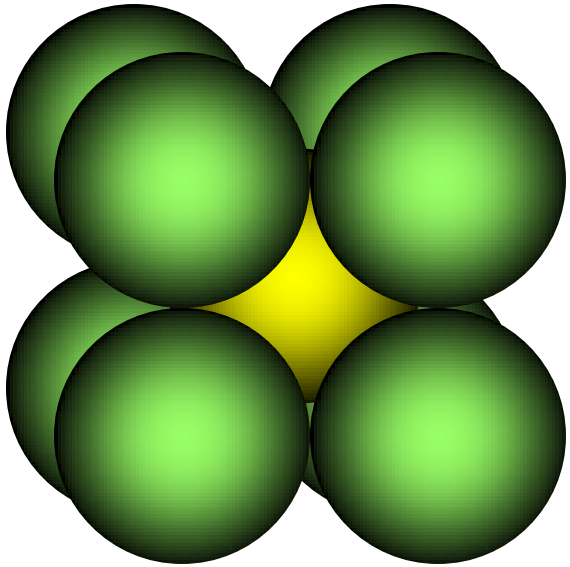
1. SIMPLE CUBIC (SC)



2. BODY CENTERED CUBIC (BCC)



2. BODY CENTERED CUBIC (BCC)



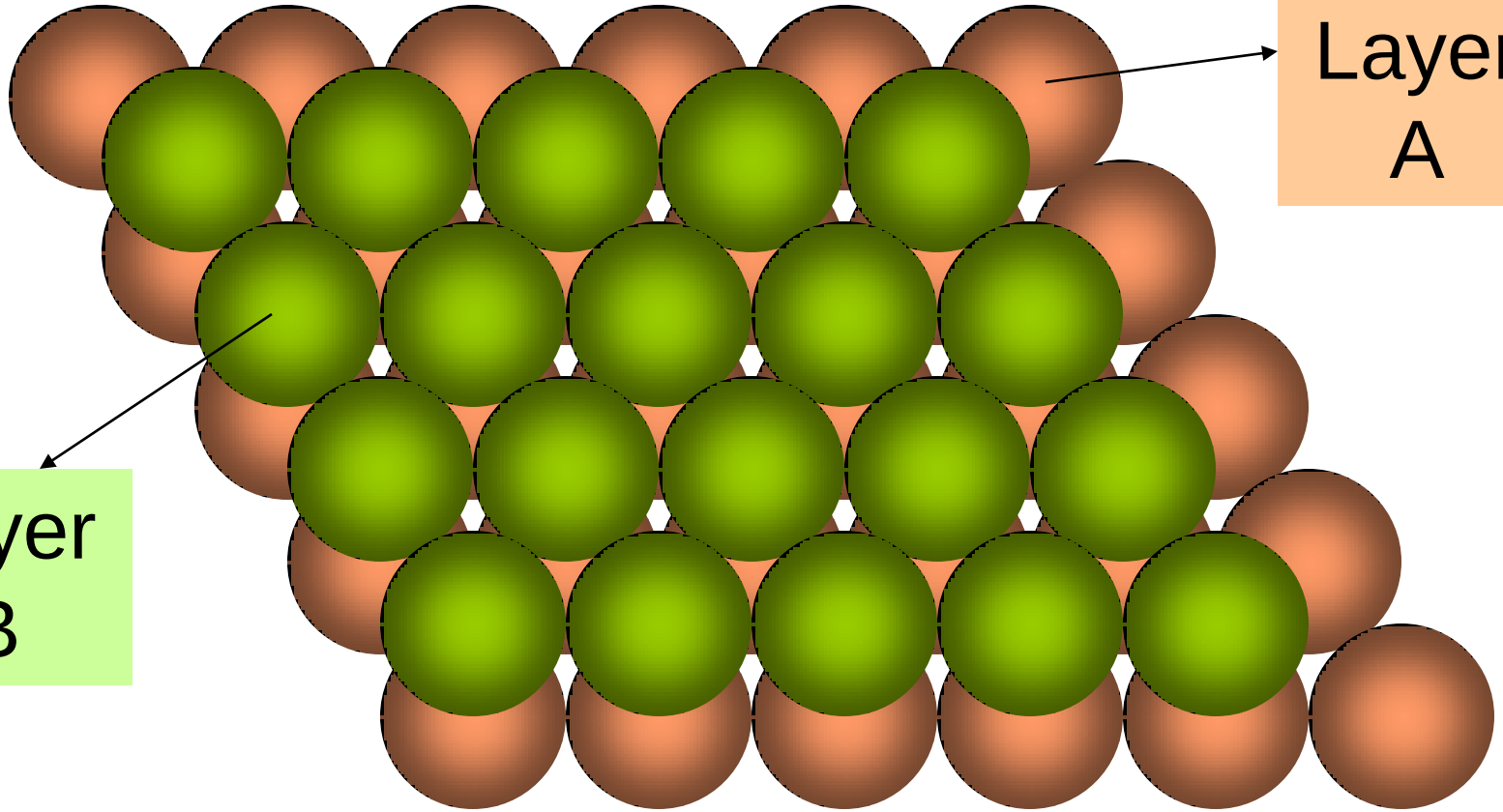
Hexagonal packing

Expanding of hexagonal packing types

1. HEXAGONAL CLOSE PACKING (HCP)

2. CUBIC CLOSE PACKING (CCP or FCC)

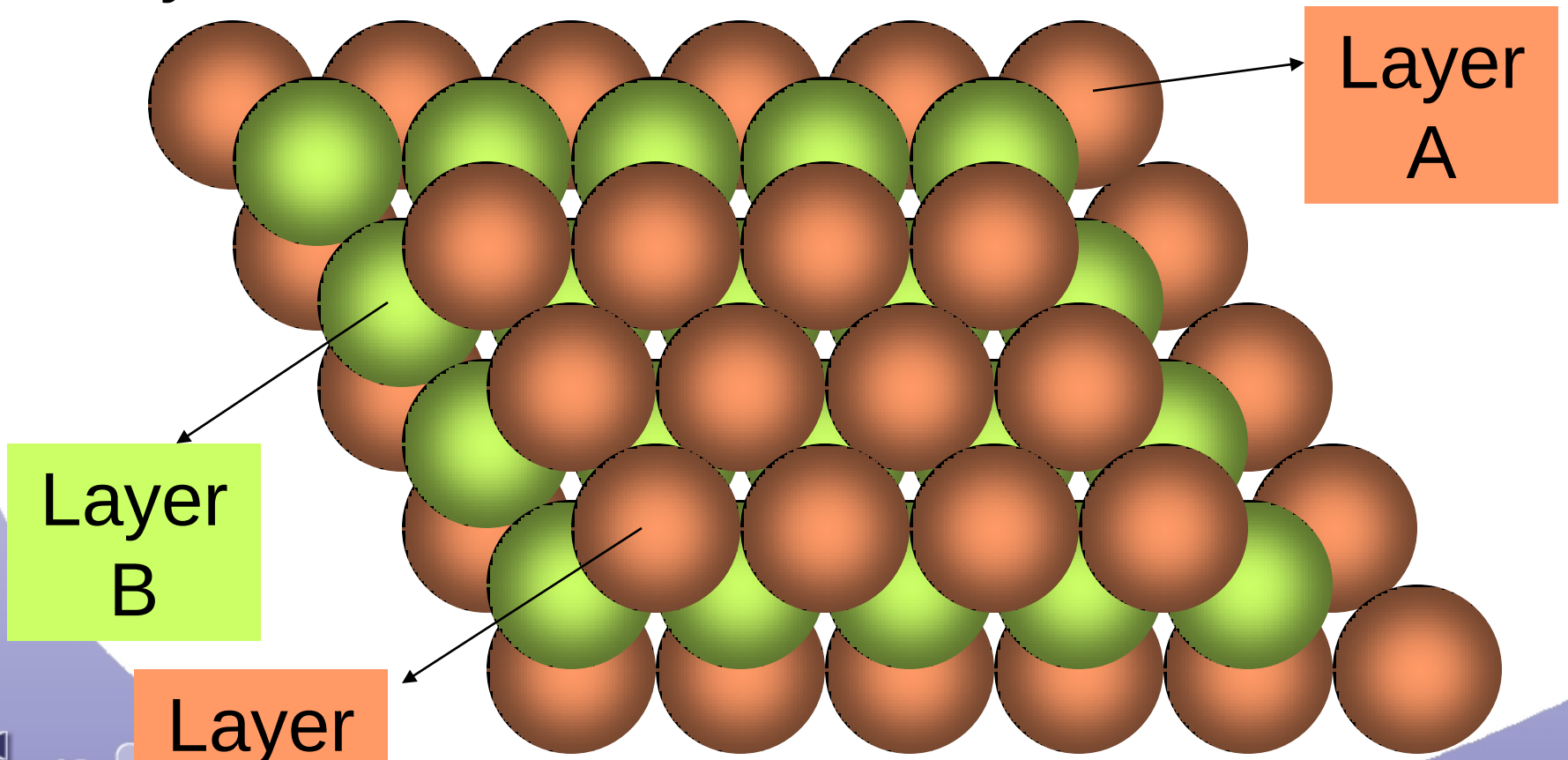
Close Packing First and Second Layers



Third layer can then be added in 2 ways:

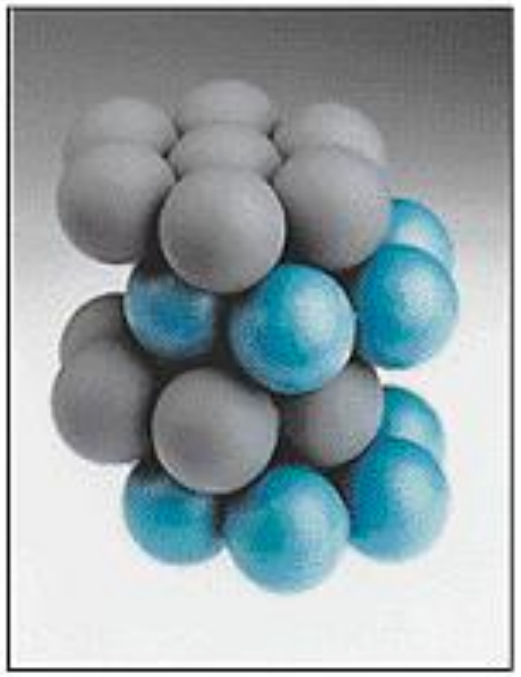
1. Hexagonal Close Packing (HCP)

- The third layer fits into the holes of the B layer such that the atoms lie above those in layer A.



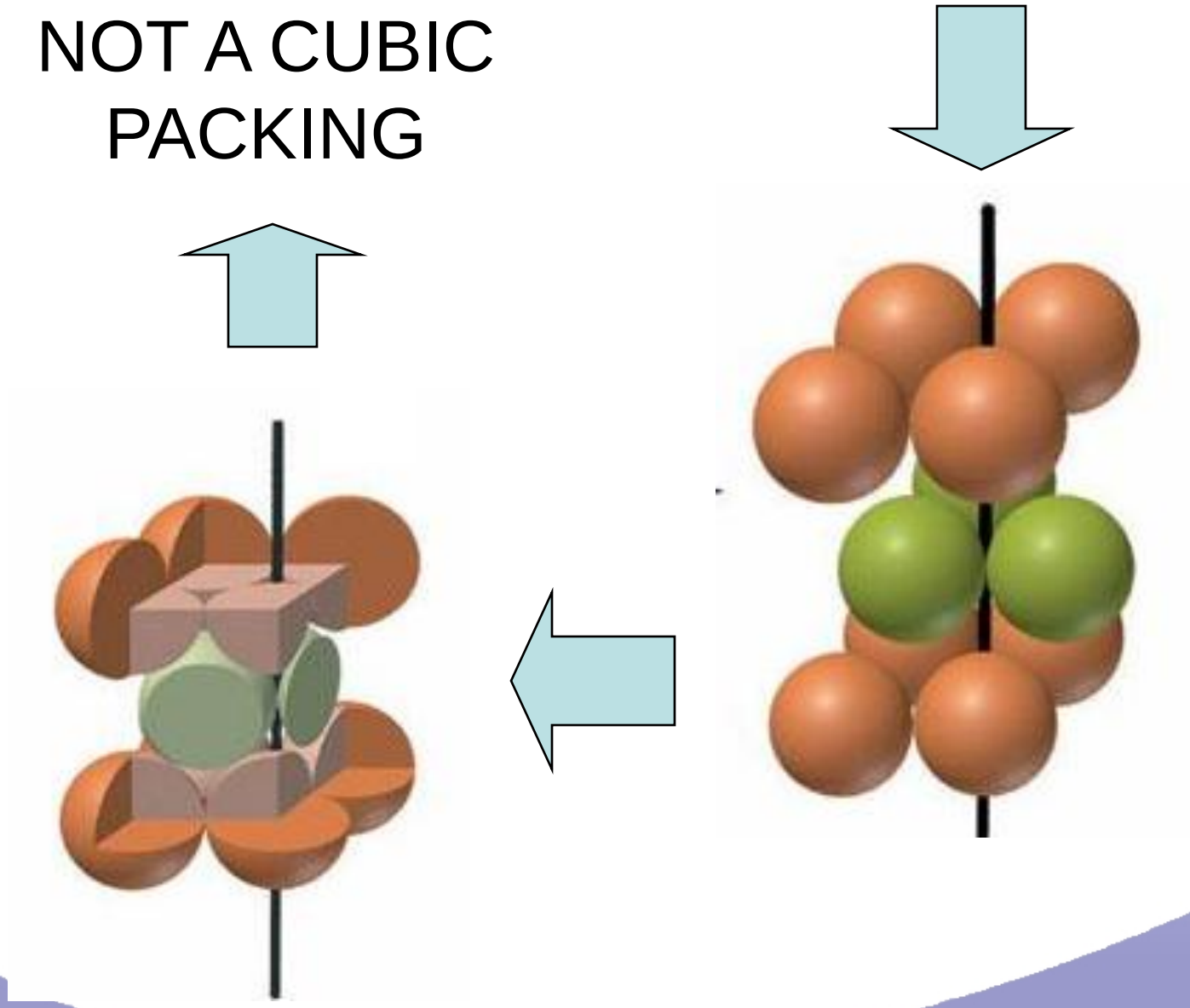
1. Hexagonal Close Packing (HCP)

By repeating this arrangement one obtains ABABAB... hexagonal closest packing



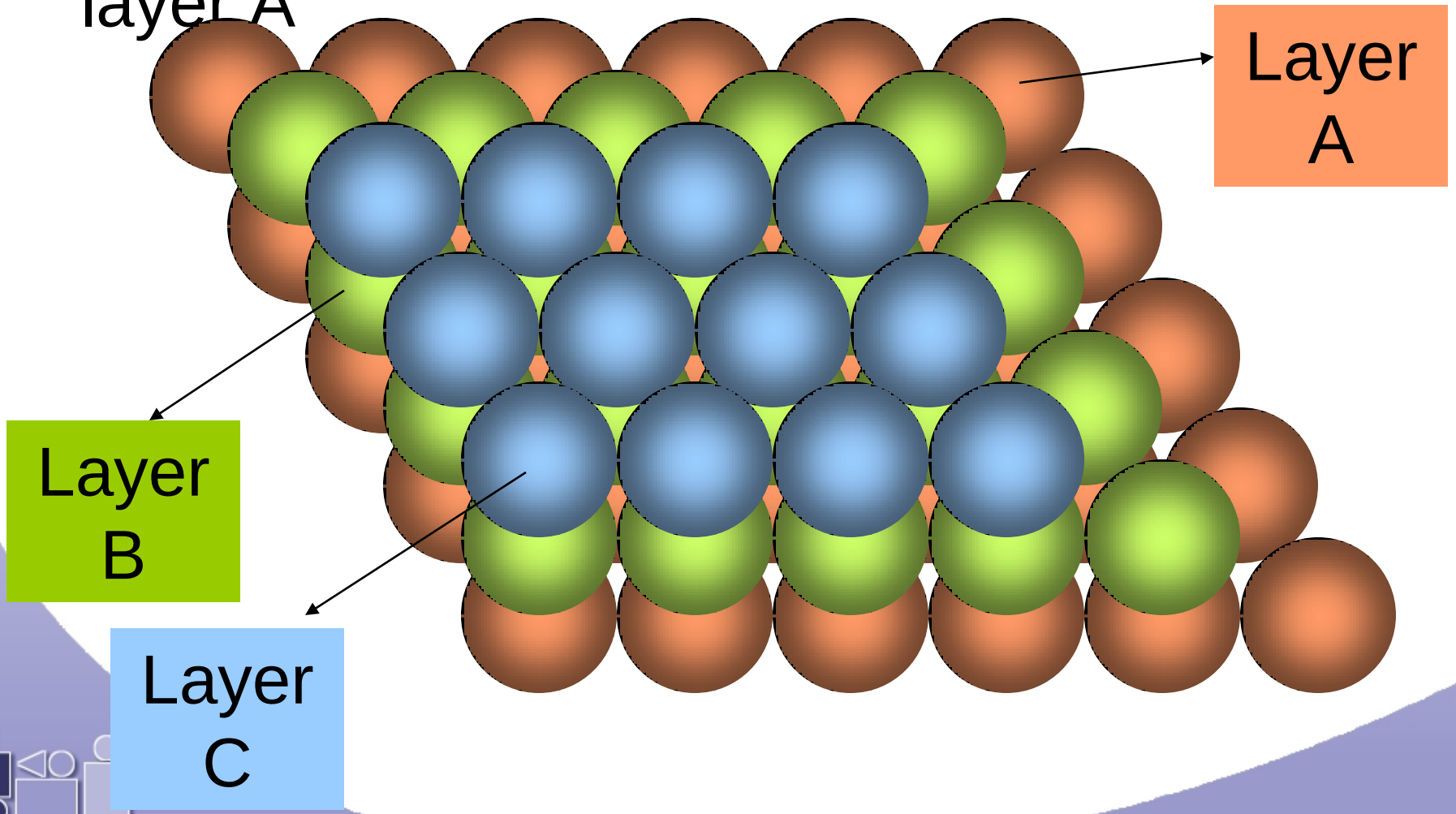
1. Hexagonal Close Packing (HCP)

NOT A CUBIC PACKING



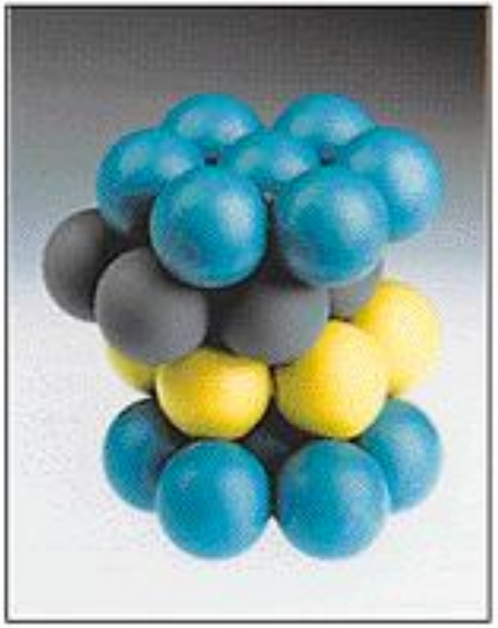
2.Cubic Close Packing (CCP or FCC)

- The third layer fits into the holes of the B and the atoms do not lie above those in layer A



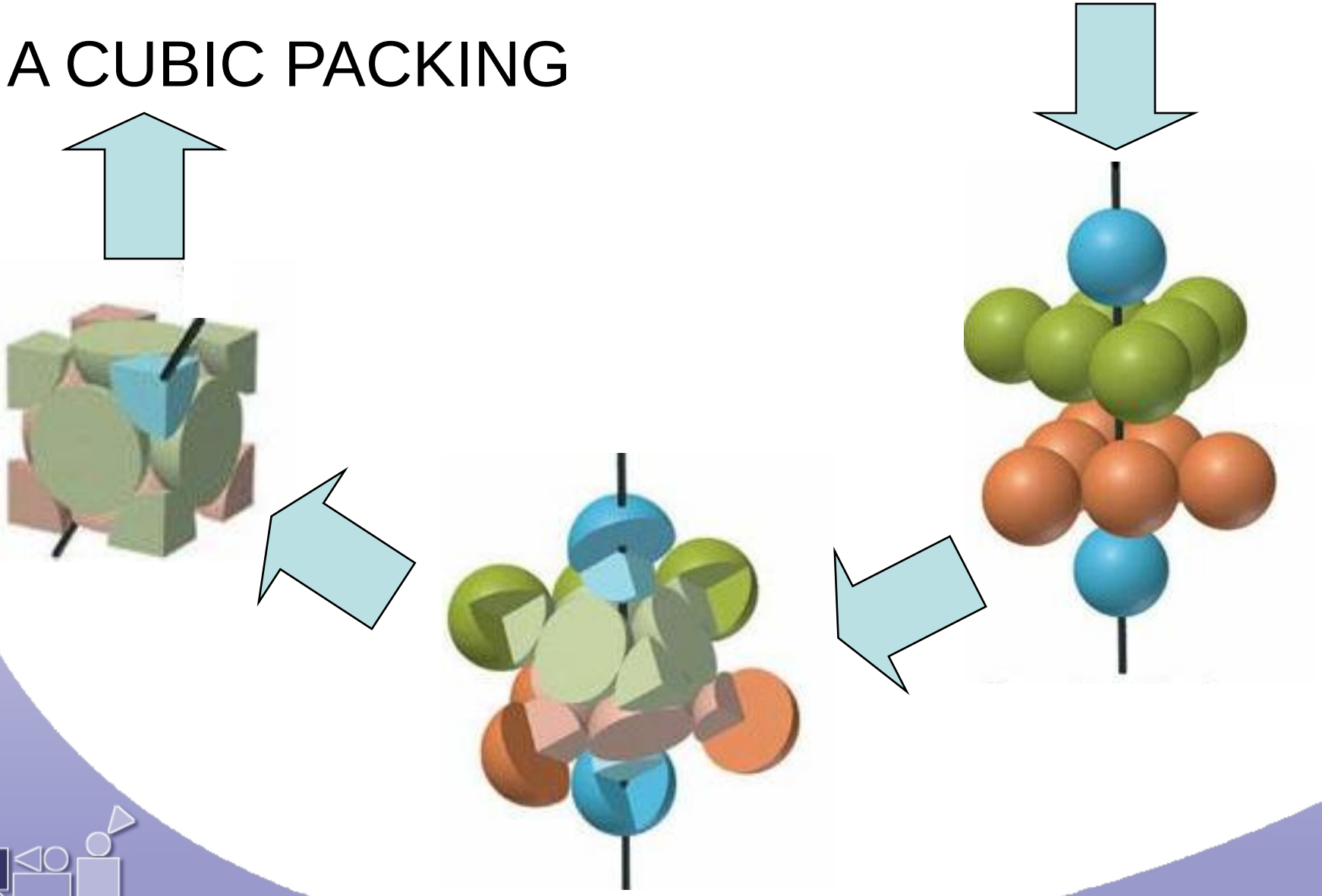
2.Cubic Close Packing (CCP or FCC)

By repeating this arrangement one obtains ABCABC..... cubic closest packing

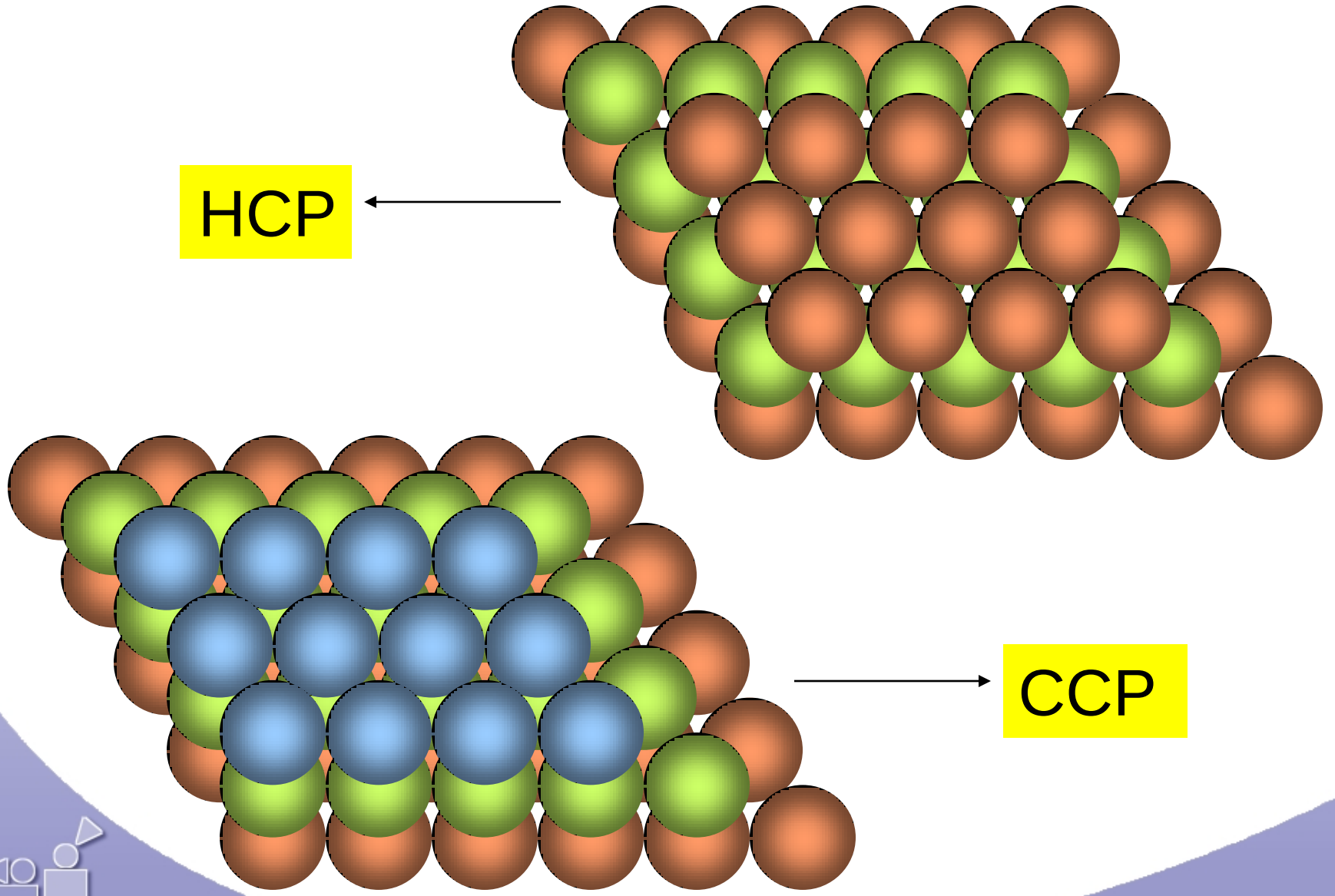


2.Cubic Close Packing (CCP or FCC)

A CUBIC PACKING

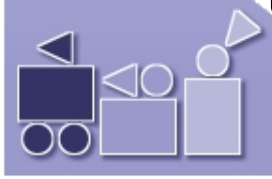


Comparison of hcp & ccp



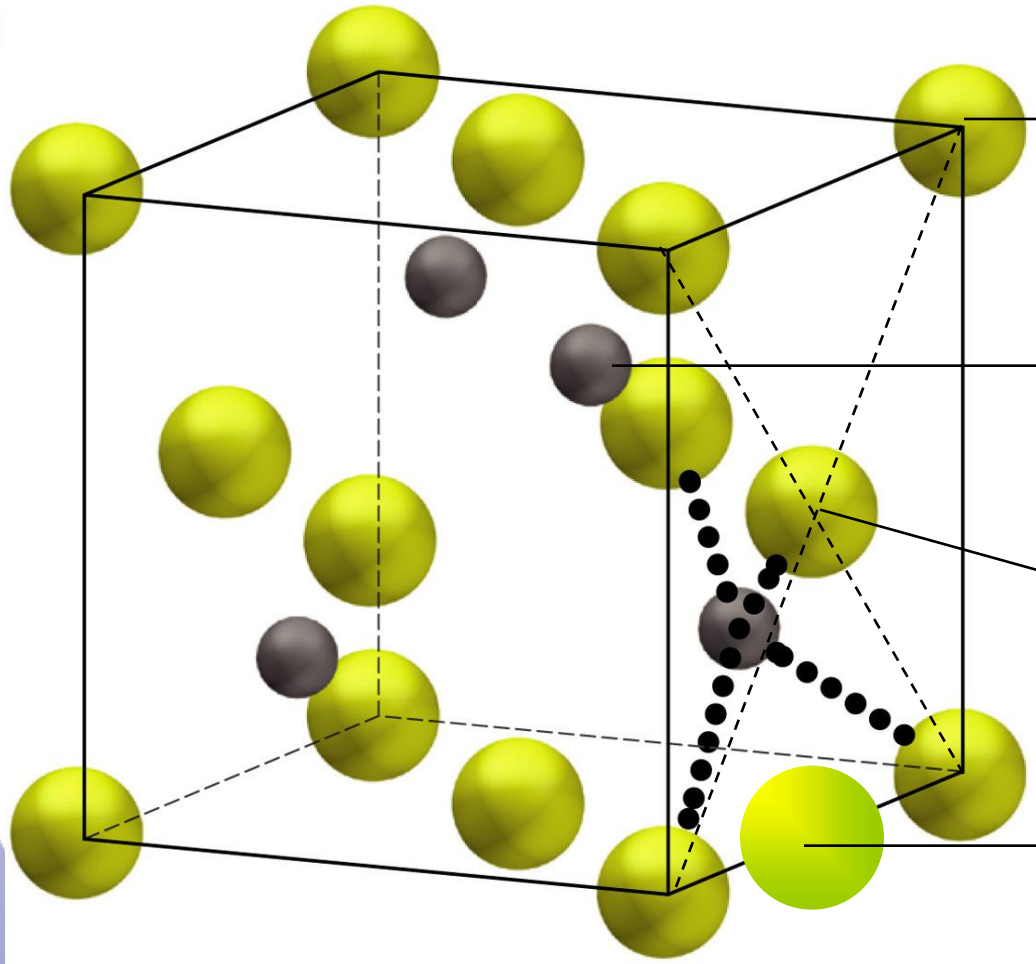
Unit Cell

- Unit cell
  - An imaginary parallel-sided region from which the entire crystal can be built up
  - Usually the smallest unit cell which exhibits the greatest symmetry is chosen.
  - If repeated (translated) in 3 dimensions, the entire crystal is recreated.



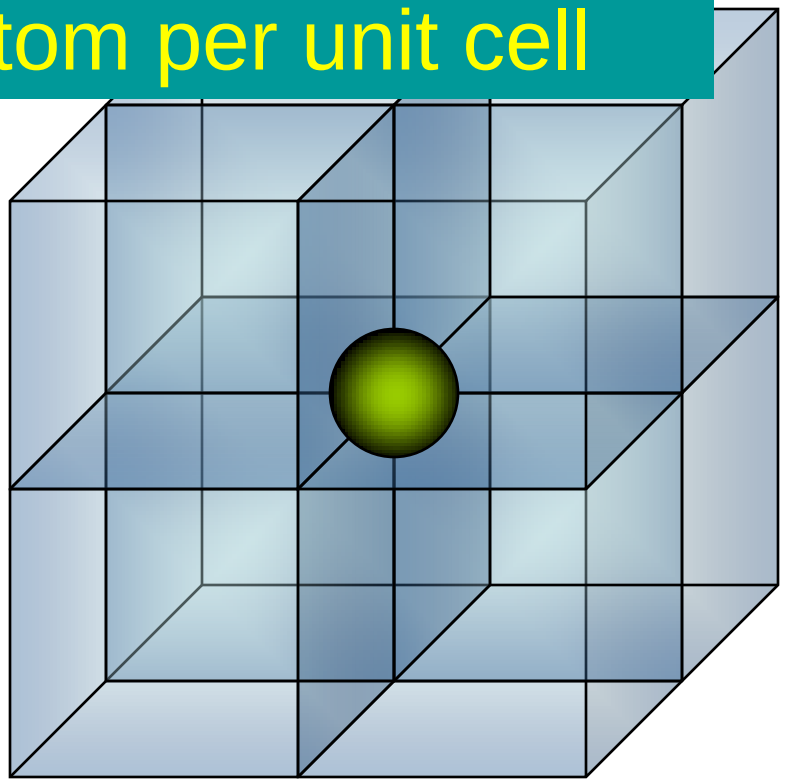
Problem 1:

- Determine the number of atom per unit cell, coordination number and packing efficiency of:
  - Simple cubic (SC)
  - Body center cubic (BCC)
  - Face center cubic (FCC)


Corner atom
Interior atom
Face atom
Site atom

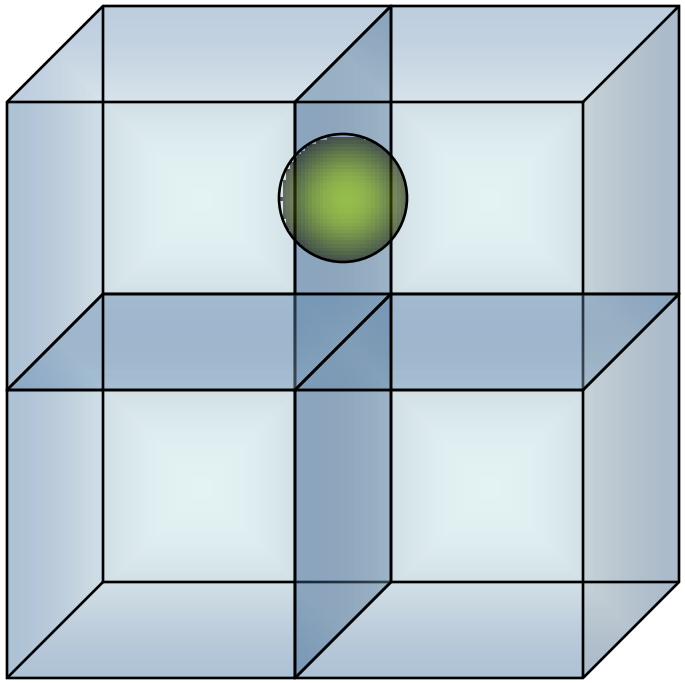
Corner atom

Corner atom = 1/8 atom per unit cell



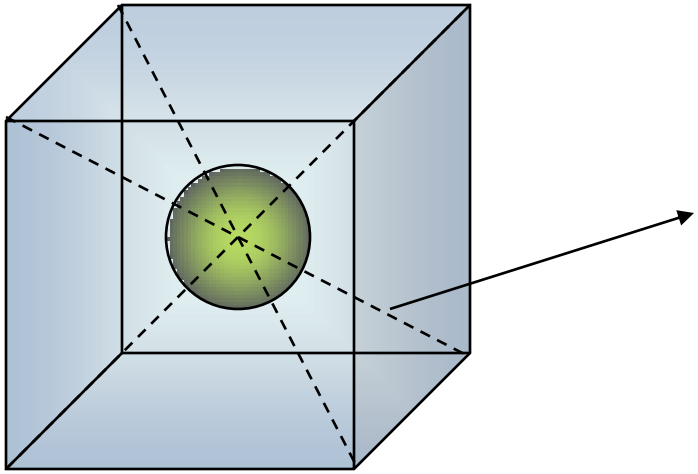
Face atom

Face atom = 1/2 atom per unit cell



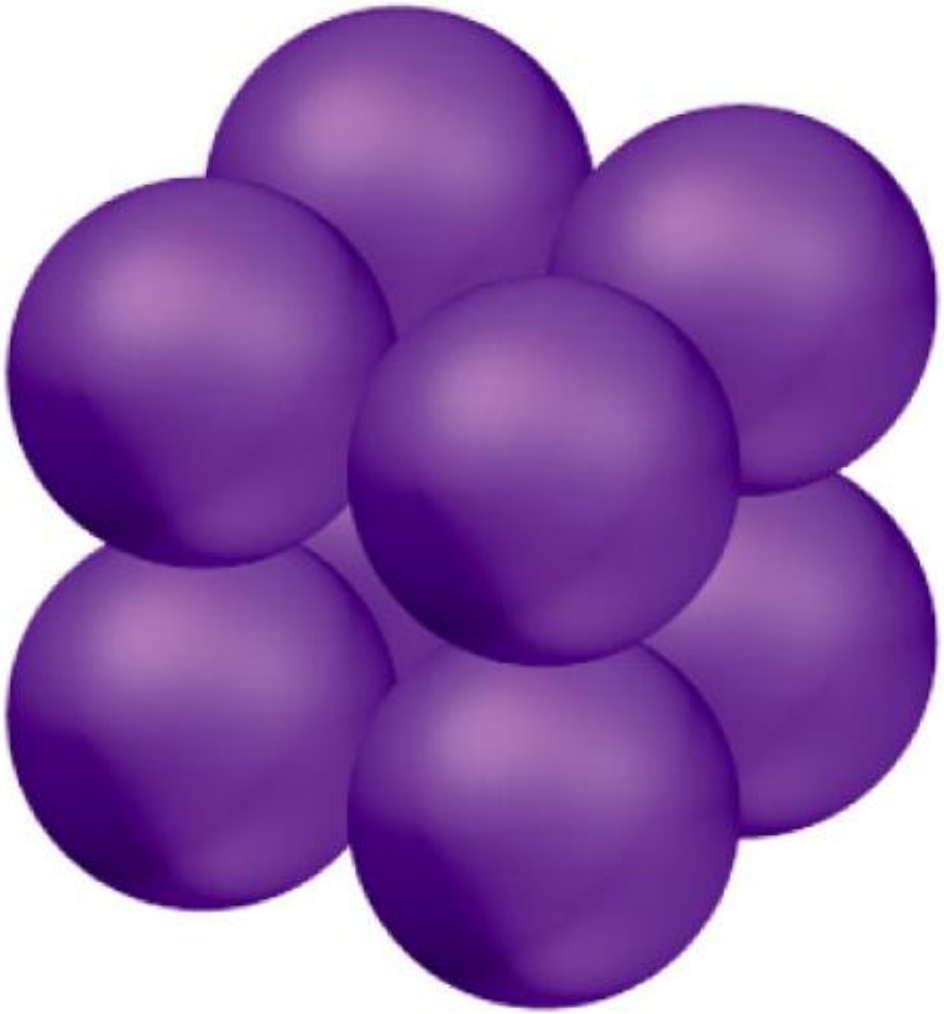
Interior atom

Interior atom = 1 atom per unit cell

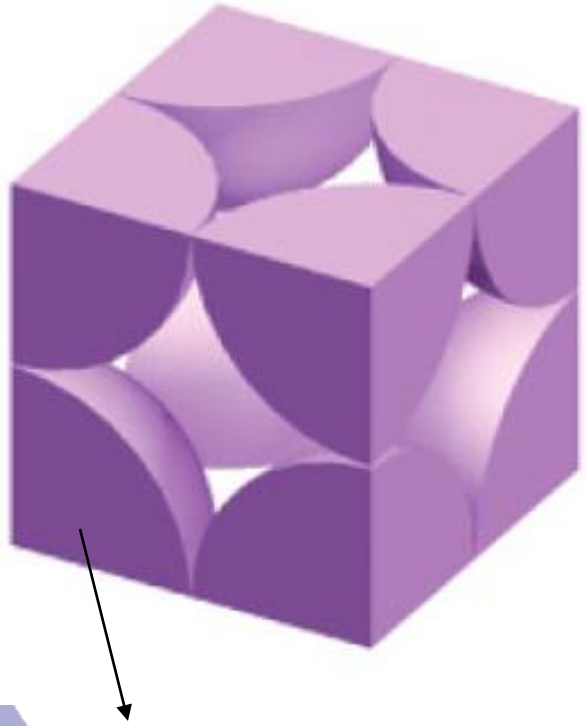


Body diagonal

Number of Atoms in SC Unit Cell



Number of Atoms in SC Unit Cell

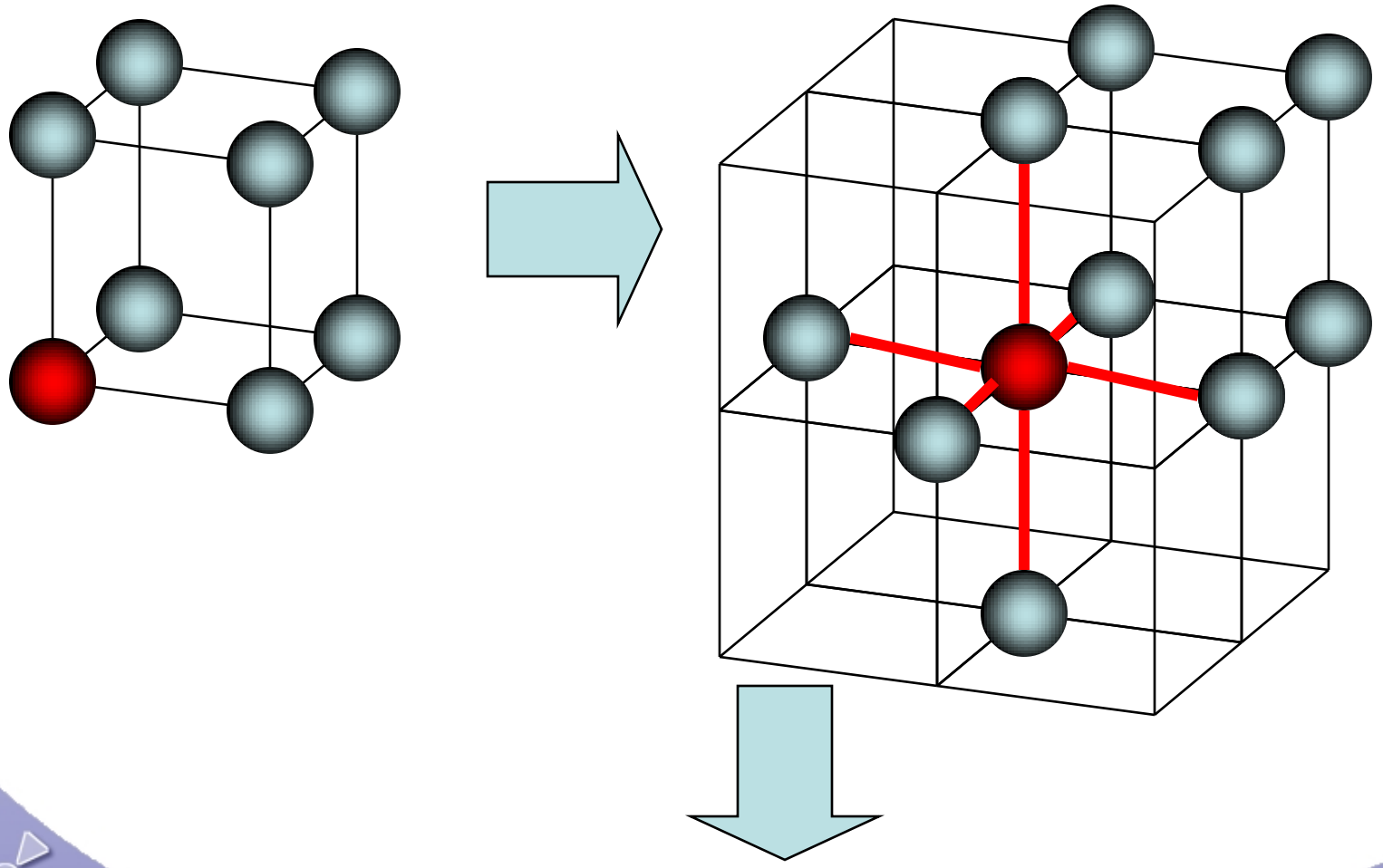


1/8 atom

$$\text{number of atom} = \frac{1}{8} \text{ x } 8 \text{ corner atoms}$$

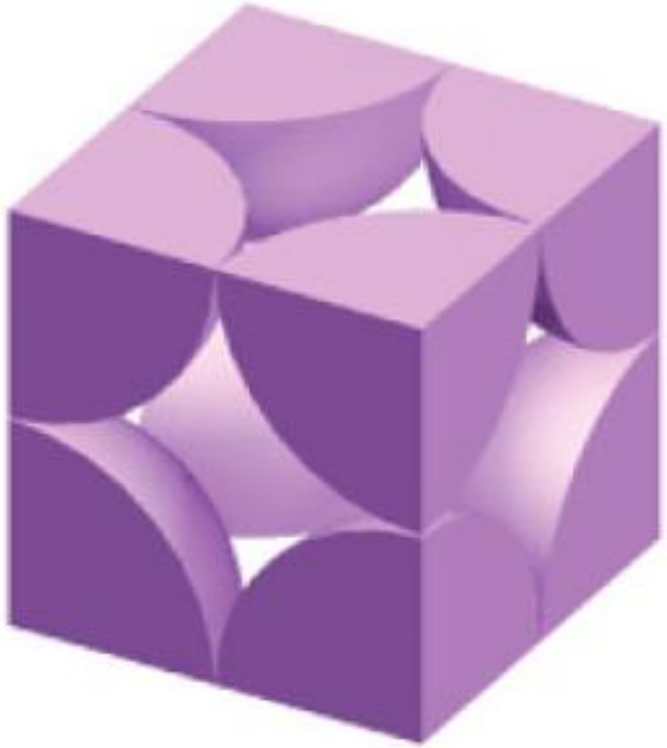
$$= 1 \text{ atom}$$

Coordination Number of SC



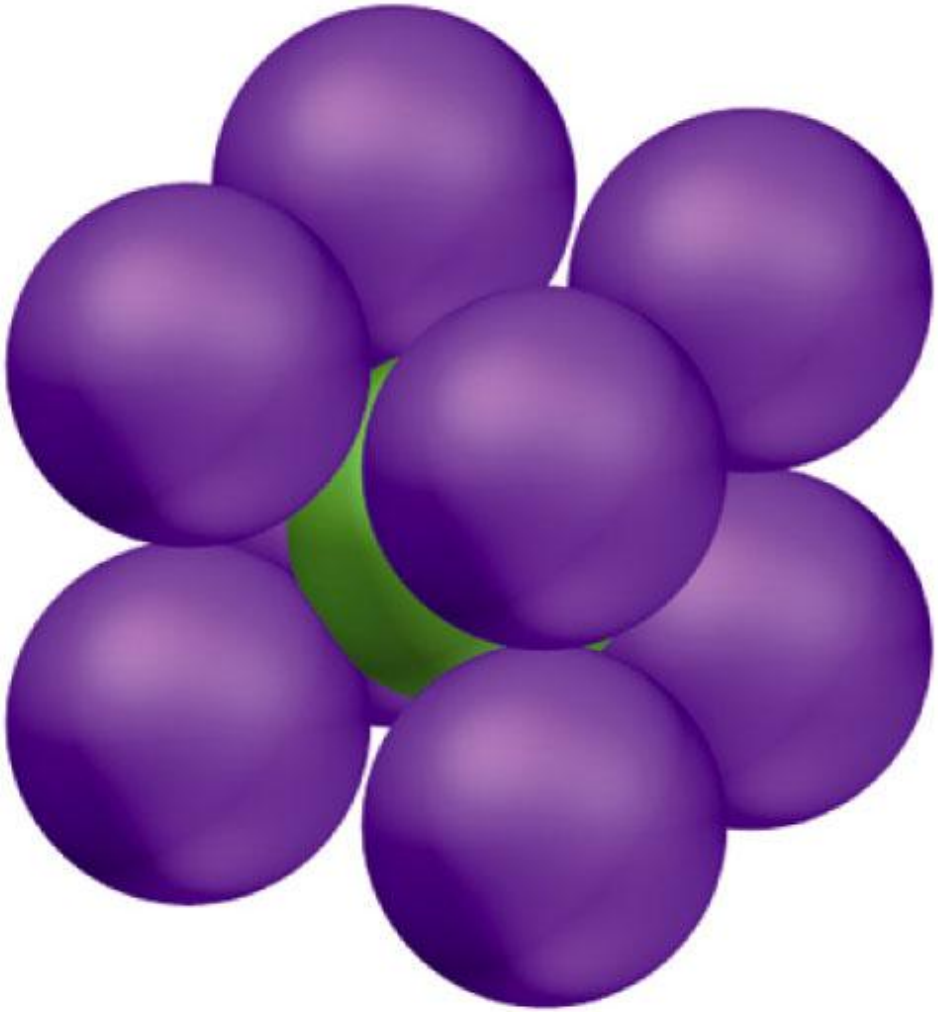
CN OF SC = 6

Packing Efficiency of SC

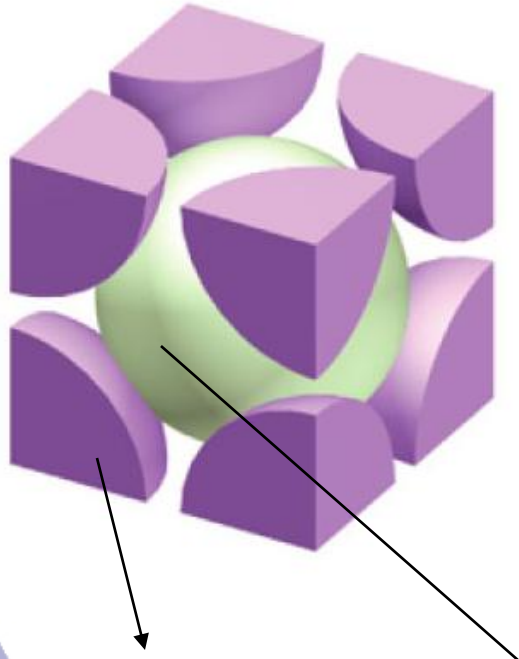


Packing efficiency = 52% ?

Number of Atoms in BCC Unit Cell



Number of Atoms in BCC Unit Cell

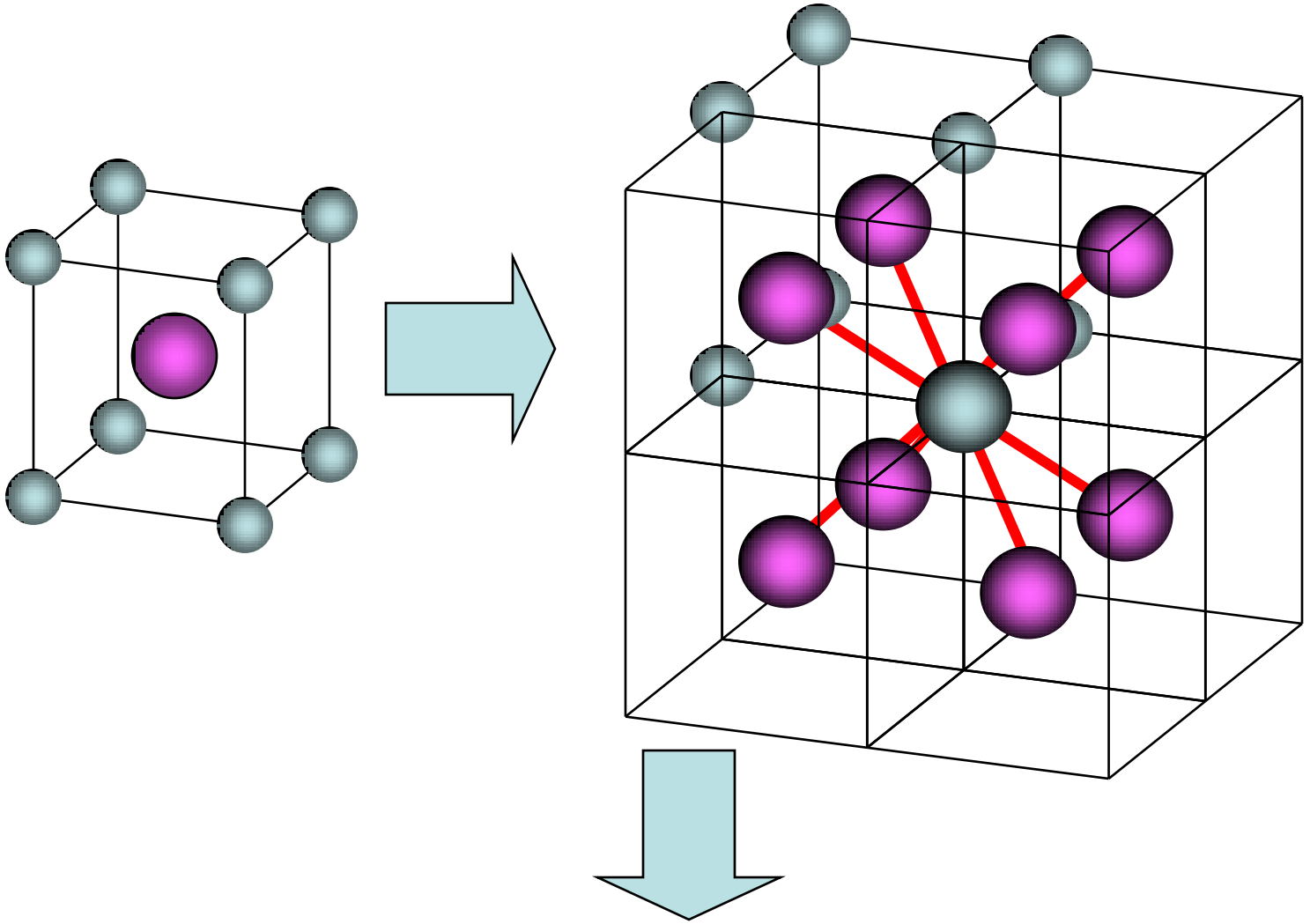


1/8 atom

1 atom

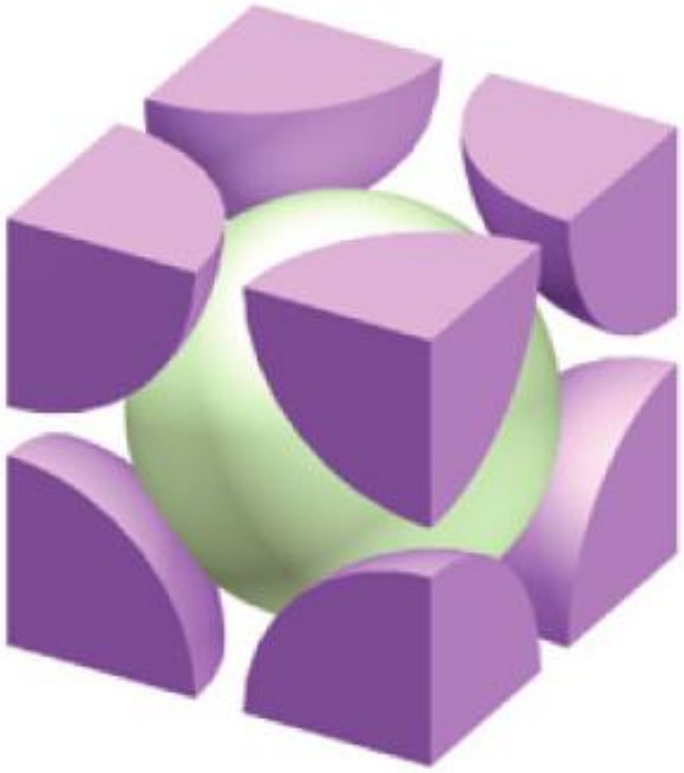
$$\text{number of atoms} = \frac{1}{8} \text{ x } 8 \text{ corner atoms}$$
$$+ 1 \text{ interior atom}$$
$$= 2 \text{ atoms}$$

Coordination Number of BCC



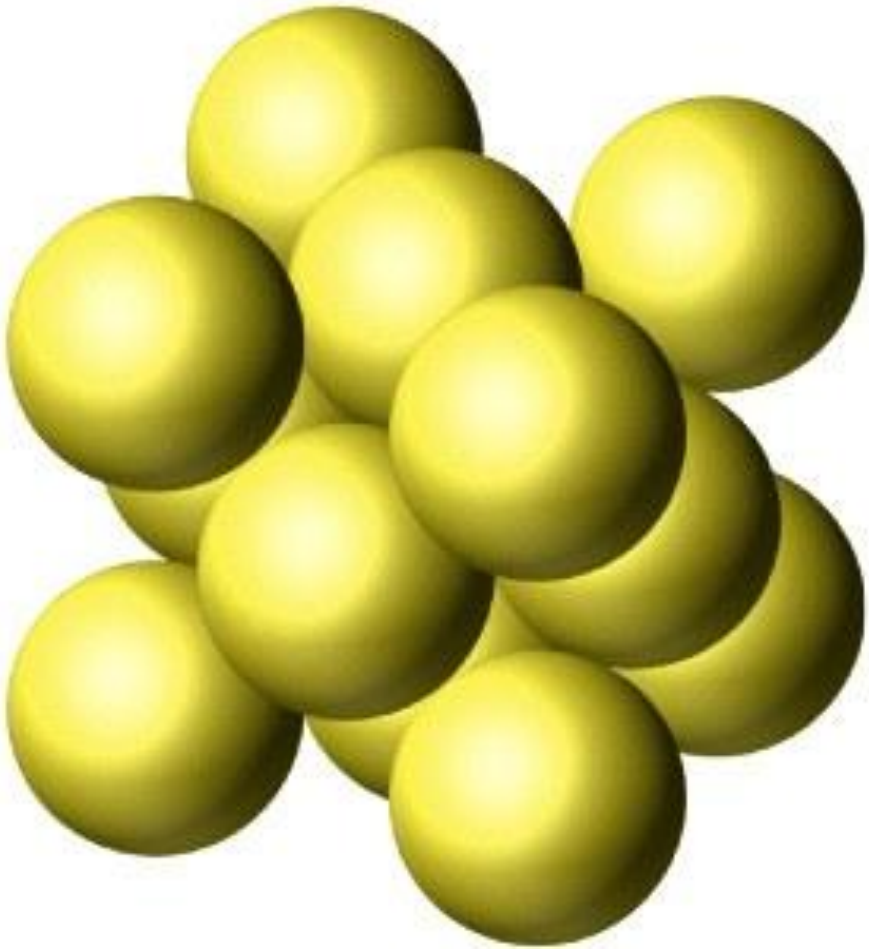
CN OF BCC = 8

Packing Efficiency of BCC

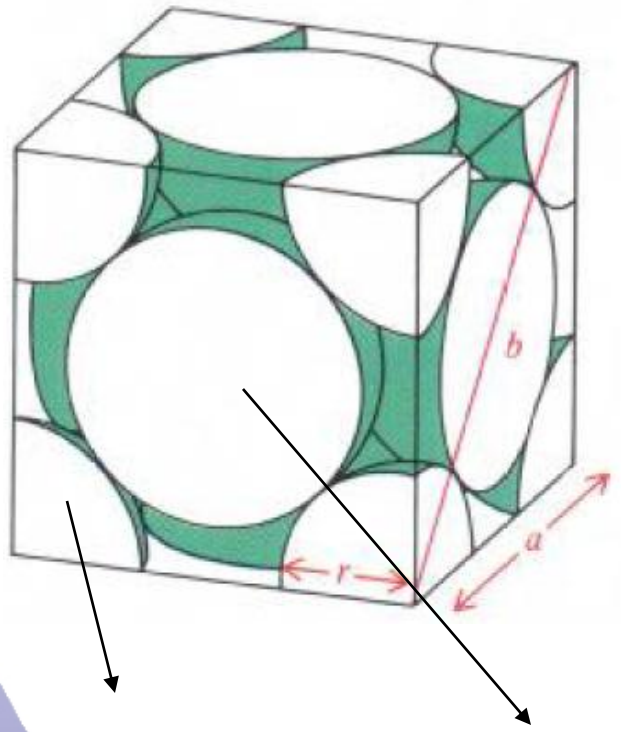


Packing efficiency = 68% ?

Number of Atoms in FCC Unit Cell



Number of Atoms in FCC Unit Cell



1/8 atom

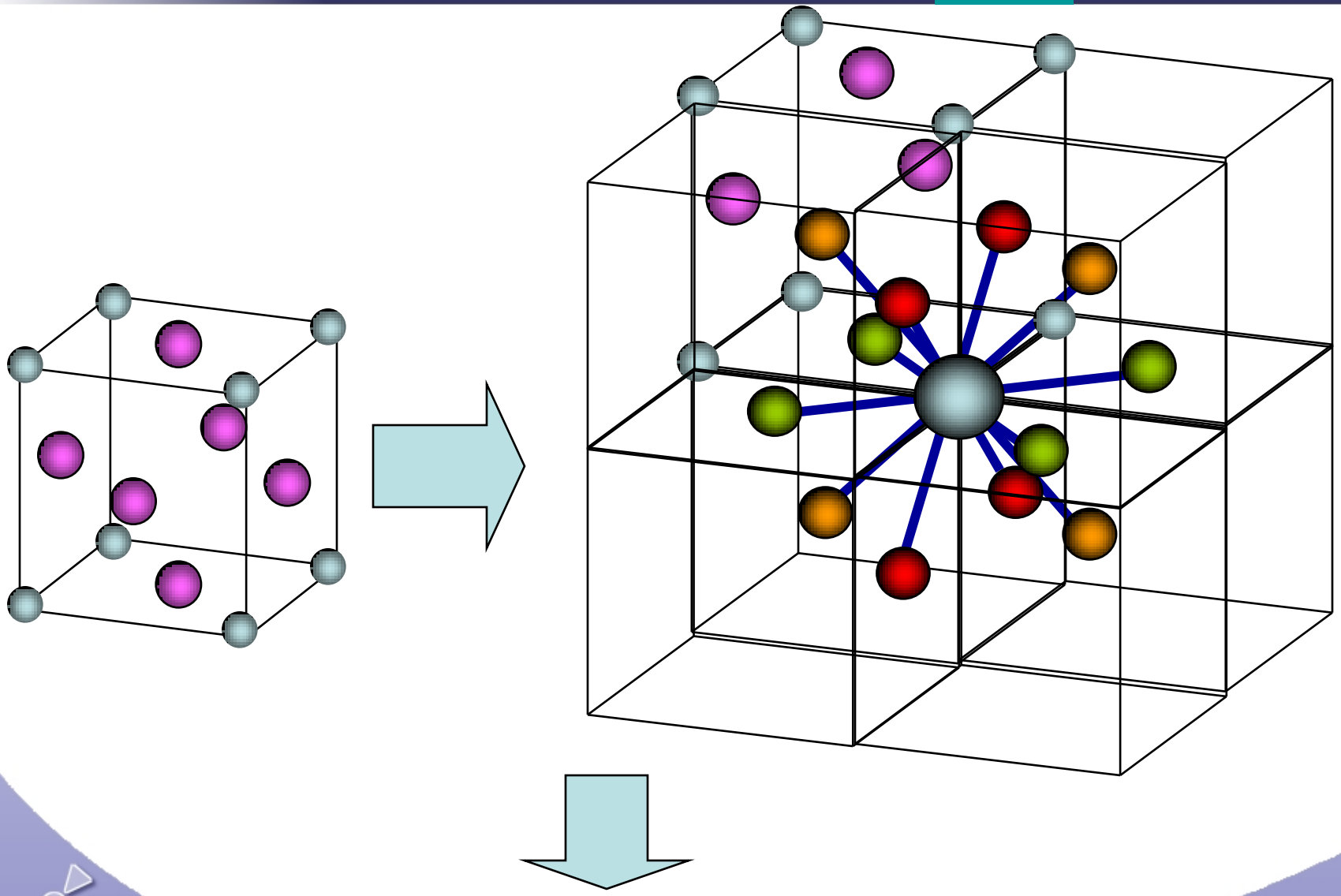
1/2 atom

$$\text{number of atoms} = \frac{1}{8} \text{ x 8 corner atoms}$$

$$+ \frac{1}{2} \text{ x 6 face atoms}$$

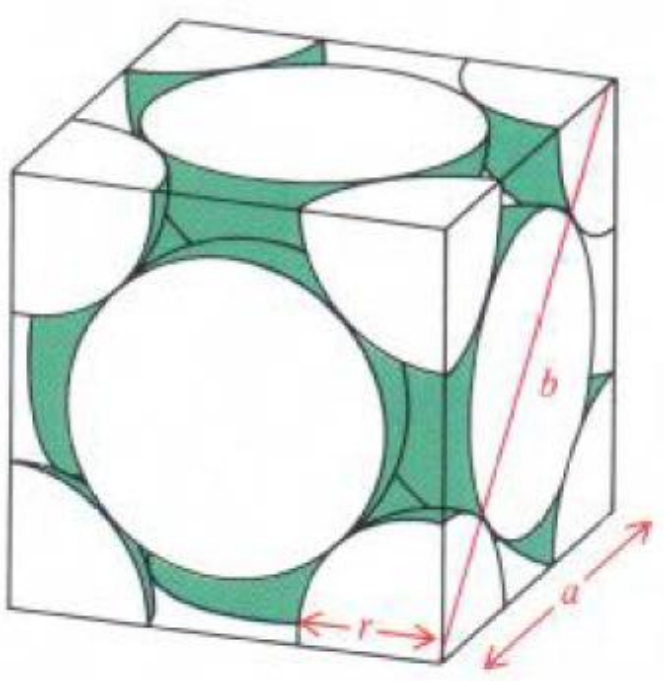
$$= 4 \text{ atoms}$$

Coordination Number of FCC



CN OF FCC = 12

Packing Efficiency of FCC



Packing efficiency = 74% ?

Keep in mind !!!

Crystal lattice	Number of atoms	Coordination number	Lattice parameter
SC	1	6	$a = 2R$
BCC	2	8	$a\sqrt{3} = 4R$
FCC	4	12	$a\sqrt{2} = 4R$

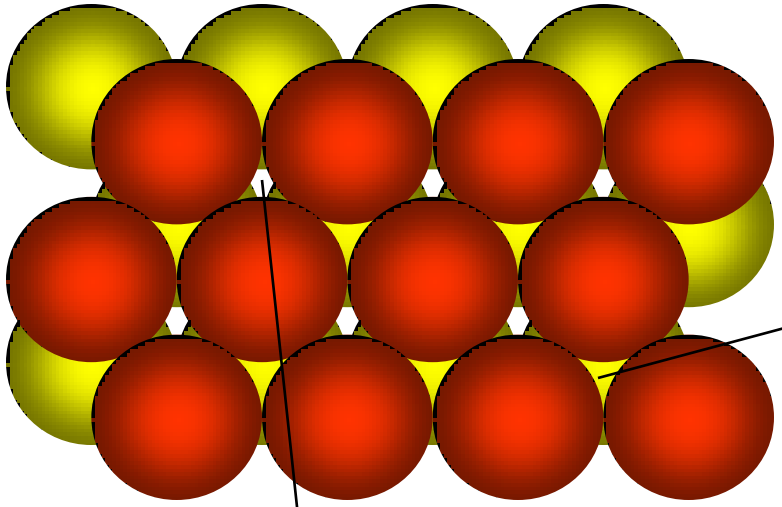
Holes in Close Packed

holes in close packed

1. TETRAHEDRAL HOLE

1. OCTAHEDRAL HOLE

Holes in Close Packed

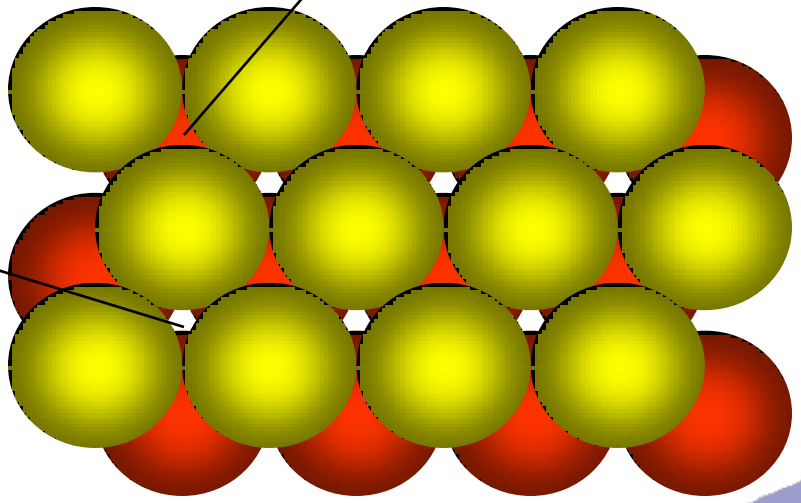


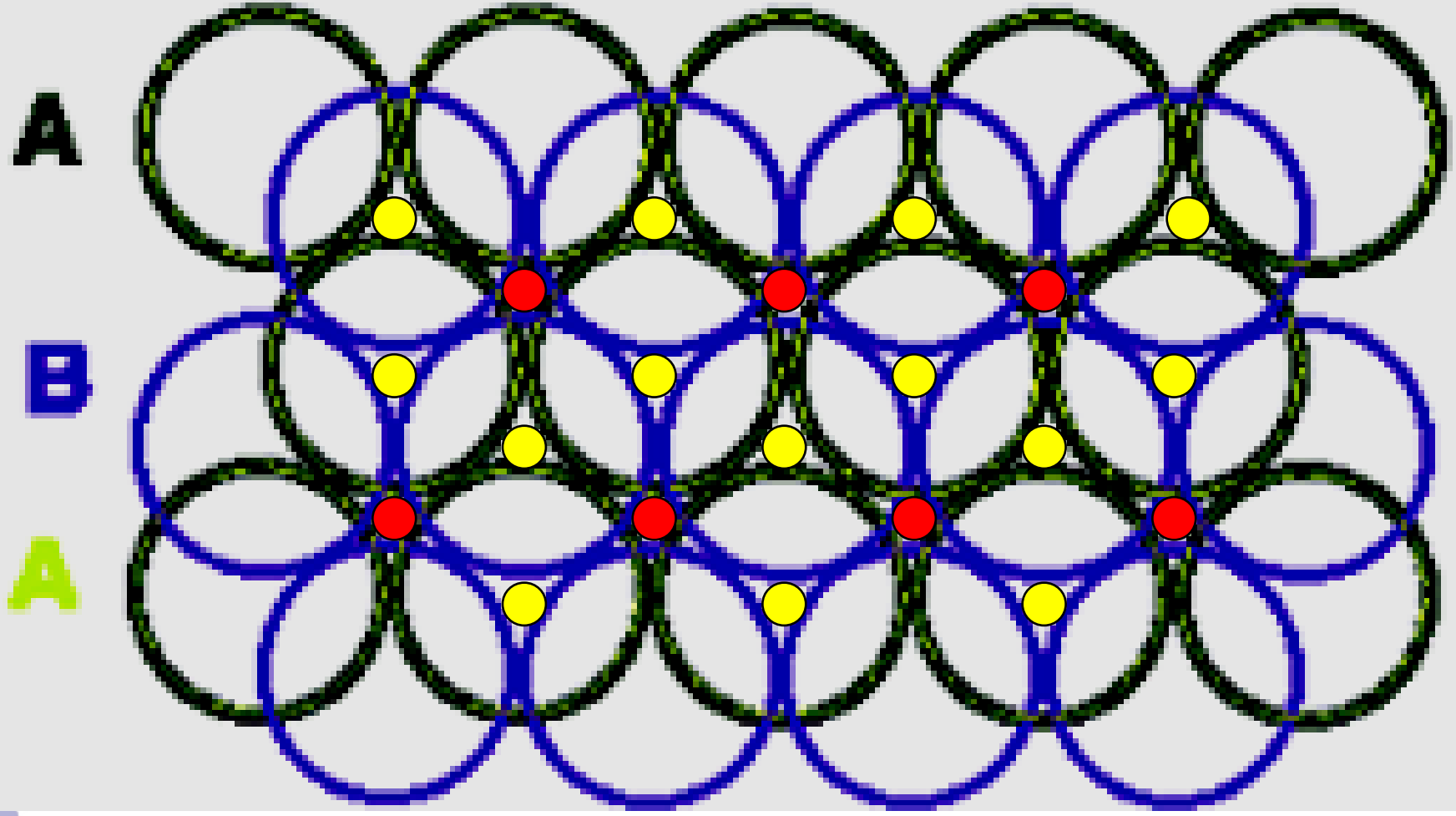
Tetrahedral hole

Different hole

Same hole

Octahedral hole

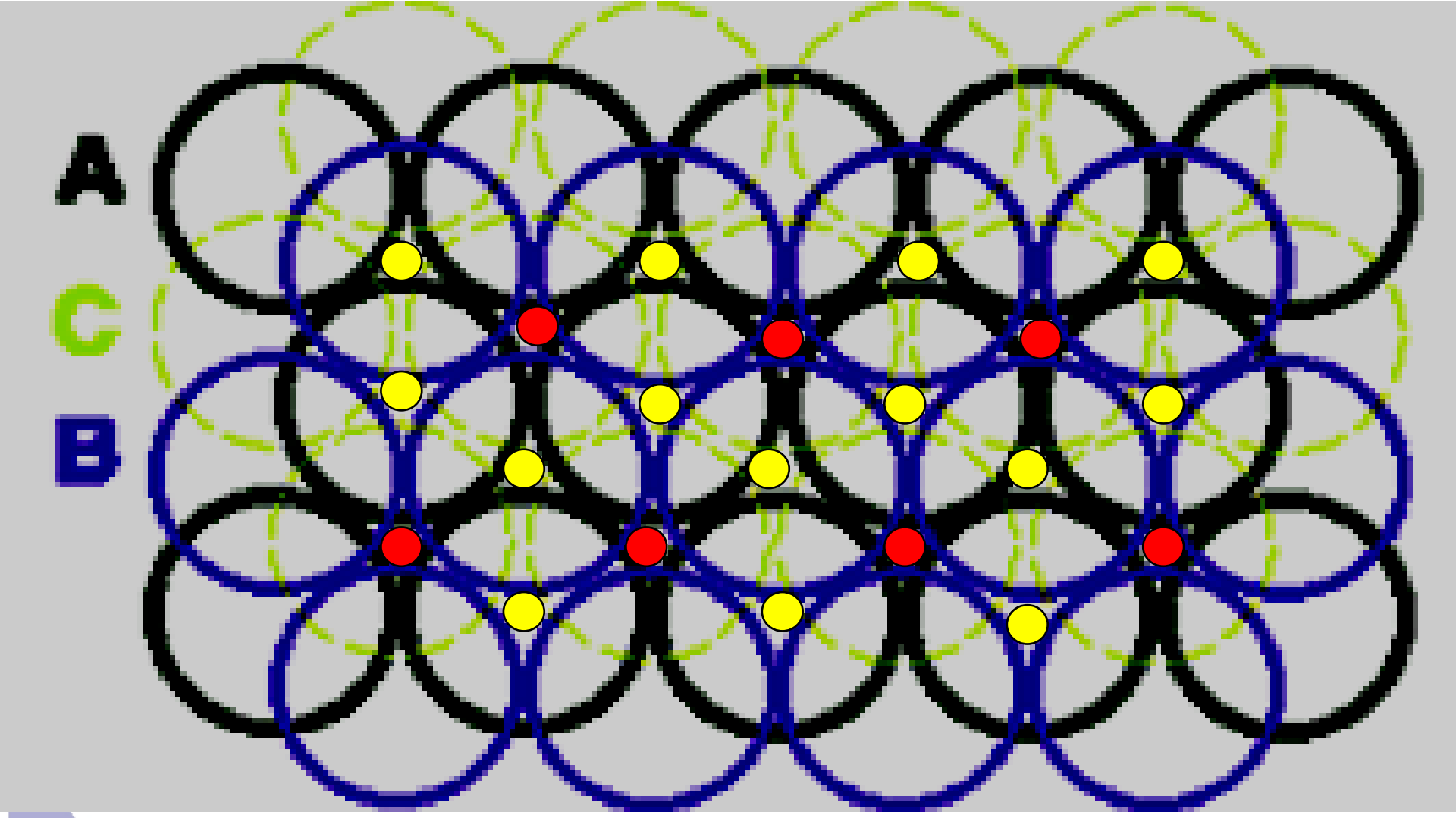




= Octahedral hole = 7

= Tetrahedral hole = 14

} tetrahedral hole 2X octahedral hole



= Octahedral hole = 7

= Tetrahedral hole = 14

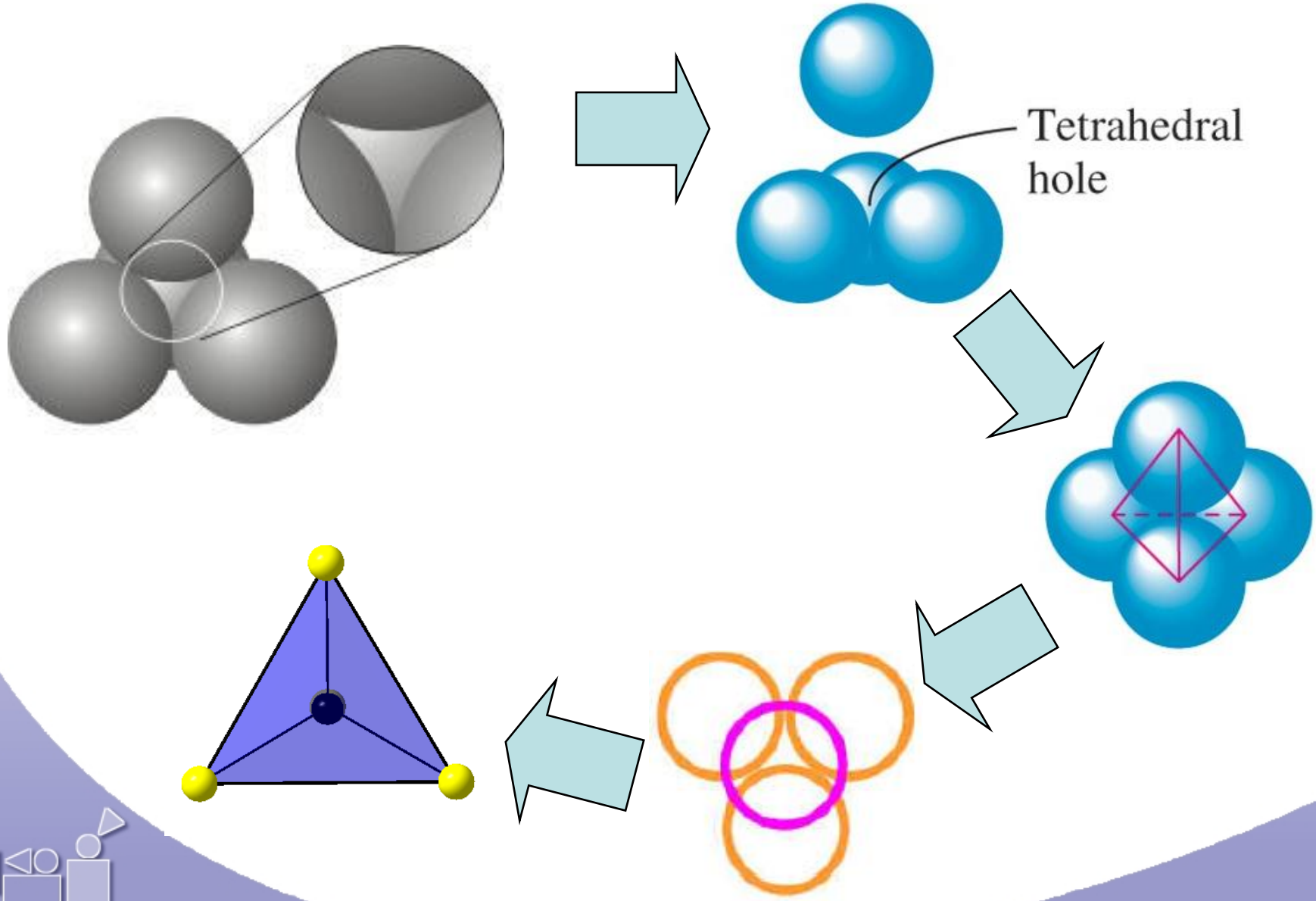
} tetrahedral hole 2X octahedral hole

Tetrahedral hole

- Formed by a planar triangle of atoms, with a 4^{th} atom covering the indentation in the center.

- The coordination number of an atom occupying an tetrahedral hole is 4.

Tetrahedral hole

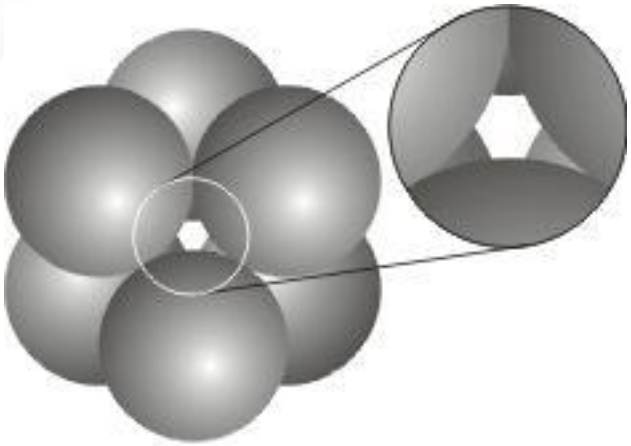


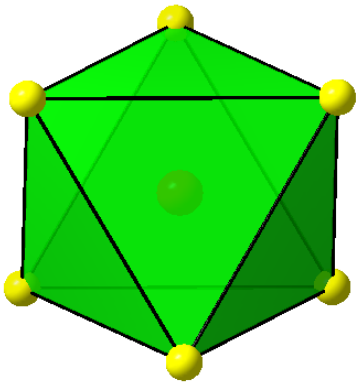
Octahedral hole

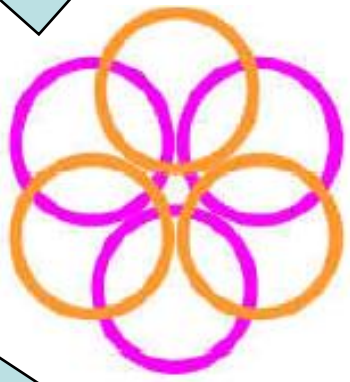
- Lies within two staggered triangular planes of atoms.

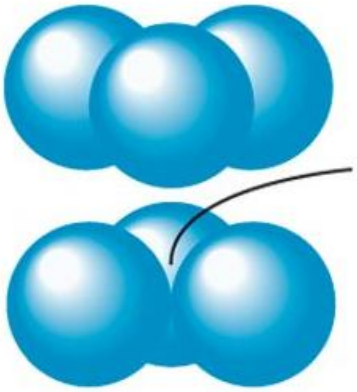
- The coordination number of an atom occupying an octahedral hole is 6.

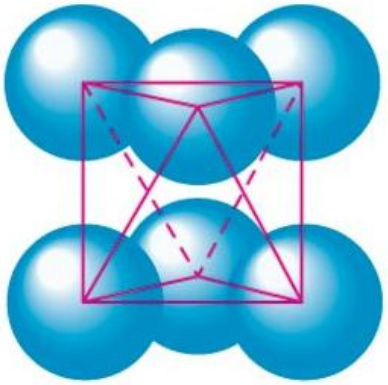
Octahedral hole











Crystal density

Crystal density determined by:

$$\rho = \frac{\Sigma\, n_i \times M}{N_A \times V}$$

Which:

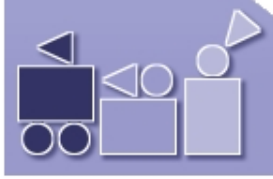
- ρ = crystal density ($g.cm^{-3}$)
- n_i = number of atoms per unit cell (atoms)
- M = molar mass of element ($gram.mol^{-1}$)
- N_A = Avogadro number (6.02×10^{23} $atoms.mol^{-1}$)
- V = volume of unit cell (cm^3)

Crystal density

Problem 2

- Calculate the density (in gram.cm^{-3})of platinum metal if it has a face centered cubic unit cell and a crystallographic radius of 135 pm (molar mass of platinum = 195.1 gram.mol^{-1})

- Answer
  - fcc = 4 atoms per unit cell
  - Lattice parameter = a
  - In fcc $\rightarrow a\sqrt{2} = 4R \rightarrow a = 2R\sqrt{2}$



– V cell $= a^3$

$= (2R\sqrt{2})^3$

$= (2 \times 135.10^{-10}. \sqrt{2})^3 \text{ cm}^3$

$= 5.567 \times 10^{-23} \text{ cm}^3$

$$\rho = \frac{\Sigma n_i \times M}{N_A \times V}$$

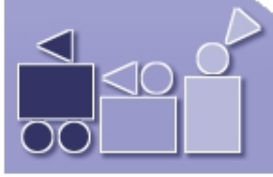
$$\rho = \frac{4 \text{ atoms} \times 195.1 \text{ gram.mol}^{-1}}{(6.02 \times 10^{23} \text{ atoms.mol}^{-1})\ (5.567 \times 10^{-23} \text{ cm}^3)}$$

$$\rho = \frac{780.4 \text{ g}}{33.513 \text{ cm}^3} = 23.28 \text{ g.cm}^{-3}$$

Problem 3

- Assume the radius of one iron atom is 1.24 angstroms (1 angstrom = 1 x 10^{-8} cm). What would be the density of body centered cubic (BCC) iron in grams/cubic centimeter? Molar mass of iron = 55.85 gram.mol^{-1}

- Hint: Find the mass and volume of one unit cell.
- Remember to count only the fraction of each atom in the cell.



- Answer
  - bcc = 2 atoms per unit cell
  - In bcc:

    $a\sqrt{3} = 4R$

    $a = 4/3\ R\ \sqrt{3}$

    $a = 4/3\ 1.24 \times 10^{-8}\ cm.\sqrt{3}$

    $= 2.86 \times 10^{-8}\ cm$

– $V_{cell} = a^3$

$= (2.86 \times 10^{-8} \text{ cm})^3$

$= 2.34 \times 10^{-23} \text{ cm}^3$

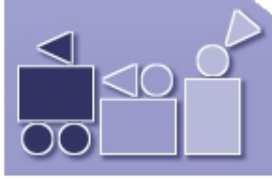
$$\text{mass of iron} = \frac{2 \text{ atoms} \times 55.85 \text{ gram.mol}^{-1}}{6.02 \times 10^{23} \text{ atom.mol}^{-1}}$$

$$= 1.85 \times 10^{-22} \text{ gram}$$

$$\rho = \frac{\text{mass}}{\text{volume}}$$

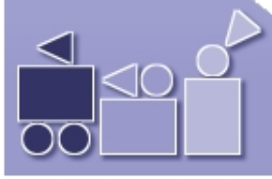
$$= \frac{1.85 \times 10^{-22} \text{ gram}}{2.34 \times 10^{-23} \text{ atom.mol}^{-1}}$$

$$= 7.91 \text{ g.cm}^{-3}$$



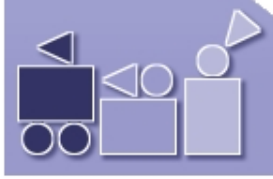
Problem 4

- Polonium (molar mass = 209 gram.mol^{-1}) metal crystallizes in a simple cubic structure.
  - Calculate the density (in gram.cm^{-3}) of the polonium metal if the atom radius is 176 pm.
  - Based on a literature density of 9.196 g cm^{-3}, what is the radius of Po(in pm)?



Problem 5

- The radius of the copper atom is 127.8 pm, and its' density is 8.95 g/cm^3. Which unit cell is consistent with these data: sc, bcc, or fcc? (molar mass of Cu = 63.55 gram.mol^{-1})



Problem 6

Below 1000°C Fe crystallizes in a body-centred cubic unit cell with an edge length of 0.28664 nm.

Above 1000°C Fe forms a face-centred cubic cell with an edge length of 0.363 nm.

- Determine the density of Fe under these conditions (in gram/cm$^{3)}$.
- Which one is denser, bcc or fcc?
- Compared to the packing efficiency, predict how it could be?

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The end of the discussion
Of
Close Packing Geometry