MLL 100

Introduction to Materials Science and Engineering

Lecture-13 (February 02, 2022)

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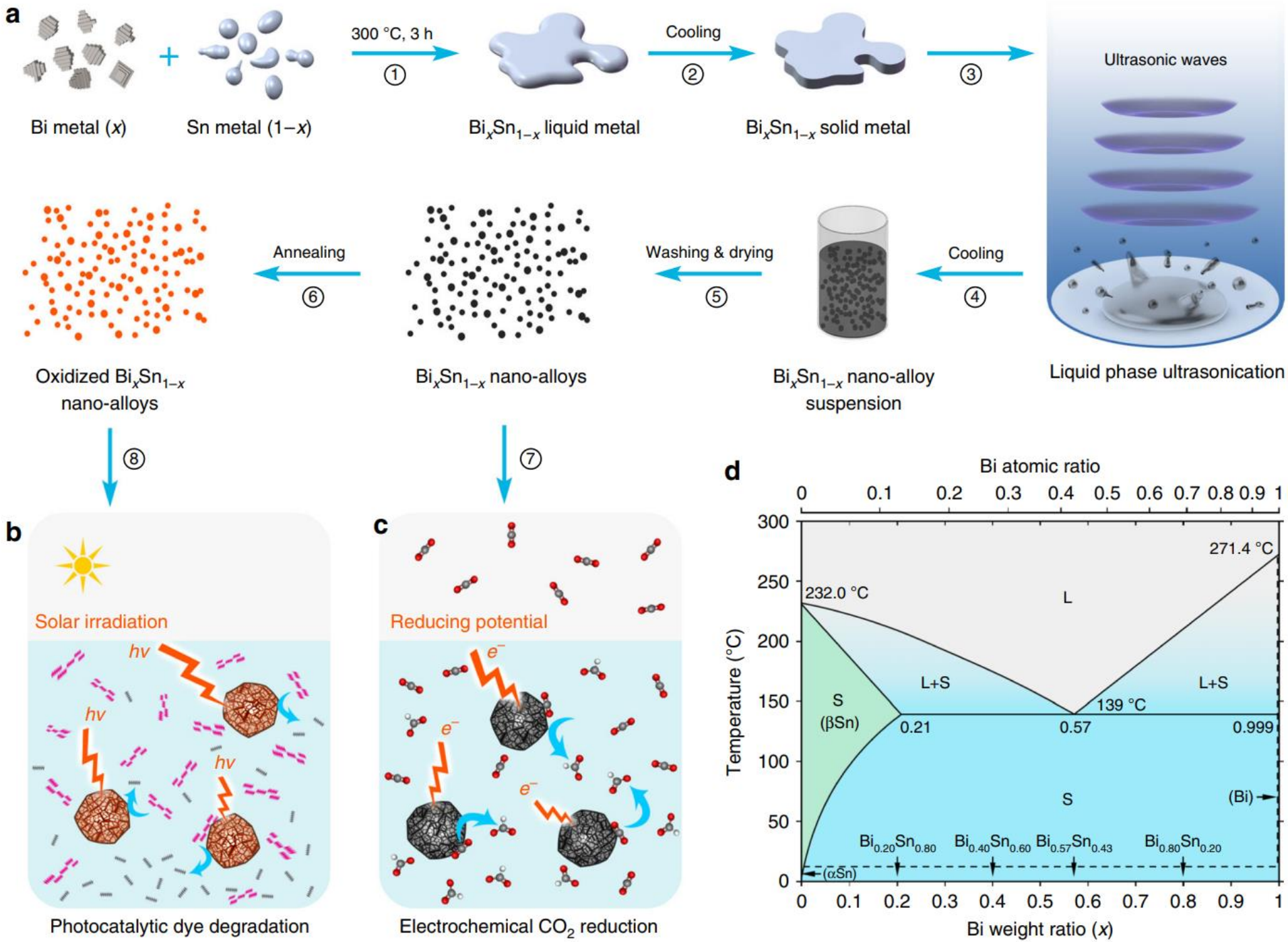
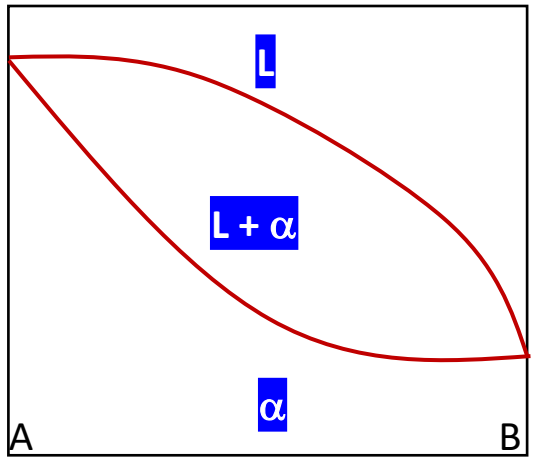
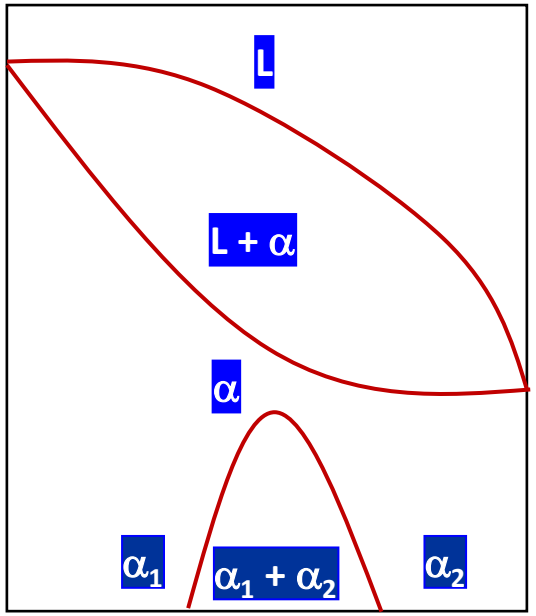
What have we learnt in Lecture-12?

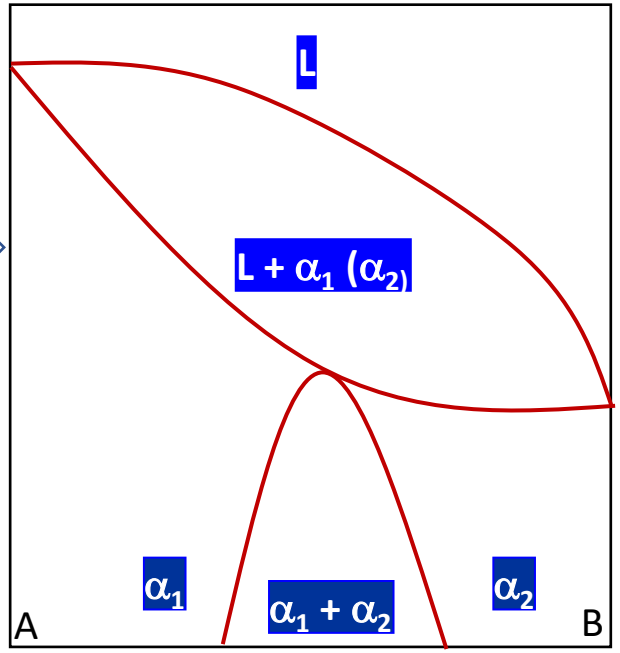
- Eutectic phase diagram

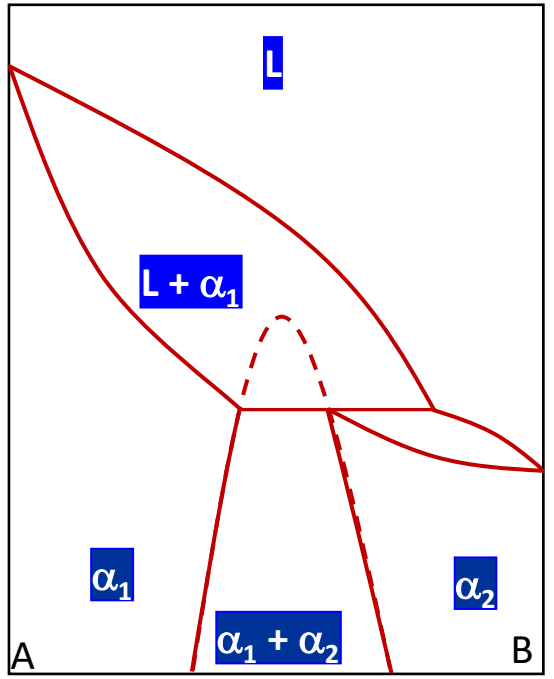

a
Bi metal (x)
Sn metal (1−x)
300 °C, 3 h
①
Bi$_x$Sn$_{1-x}$ liquid metal
Cooling
②
Bi$_x$Sn$_{1-x}$ solid metal
③
Ultrasonic waves
Liquid phase ultrasonication
Cooling
④
Bi$_x$Sn$_{1-x}$ nano-alloy suspension
Washing & drying
⑤
Bi$_x$Sn$_{1-x}$ nano-alloys
Annealing
⑥
Oxidized Bi$_x$Sn$_{1-x}$ nano-alloys
⑦
⑧
b
Solar irradiation
hv
hv
hv
Photocatalytic dye degradation
c
Reducing potential
e⁻
e⁻
e⁻
Electrochemical CO$_2$ reduction
d
Bi atomic ratio
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Temperature (°C)
300 250 200 150 100 50 0
271.4 °C
232.0 °C
L
L+S
L+S
S
(βSn)
139 °C
0.21
0.57
0.999
S
(Bi)
Bi$_{0.20}$Sn$_{0.80}$
Bi$_{0.40}$Sn$_{0.60}$
Bi$_{0.57}$Sn$_{0.43}$
Bi$_{0.80}$Sn$_{0.20}$
(αSn)
0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
Bi weight ratio (x)

Isomorphous ⟶ Peritectic phase diagram



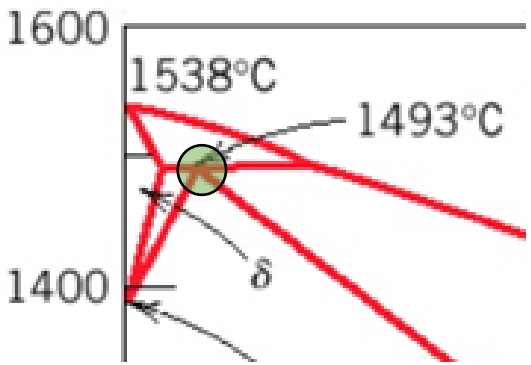






- When the melting points of the two components differ significantly, the system tends to form a peritectic phase diagram.

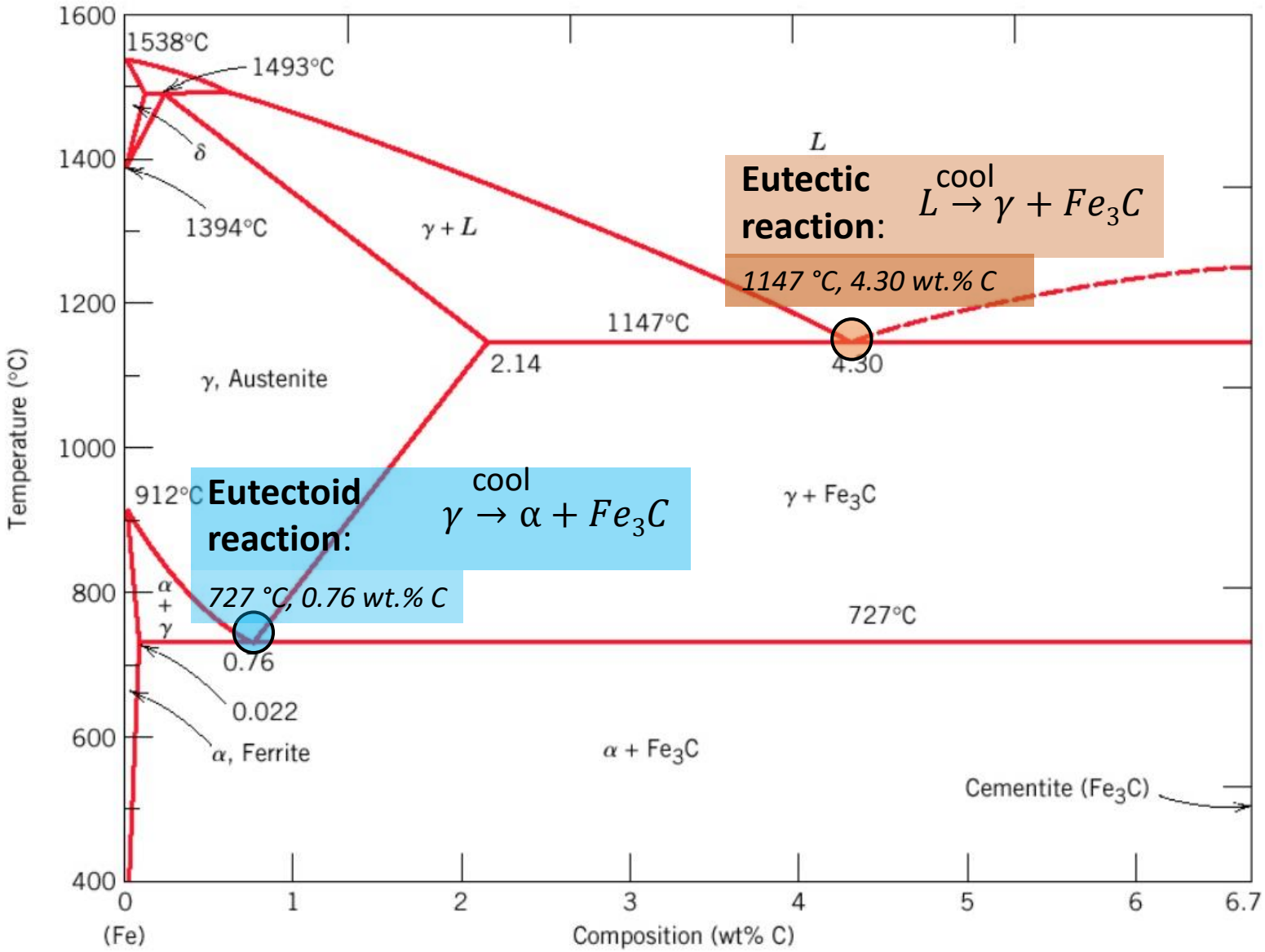
Iron-carbon phase diagram



Peritectic reaction: $L + \delta \overset{\text{cool}}{\rightarrow} \gamma$

1493 °C, 0.16 wt.% C

The 'Eutectoid reaction' holds technological significance.



Eutectic reaction: $L \overset{\text{cool}}{\rightarrow} \gamma + Fe_3C$

1147 °C, 4.30 wt.% C

Eutectoid reaction: $\gamma \overset{\text{cool}}{\rightarrow} \alpha + Fe_3C$

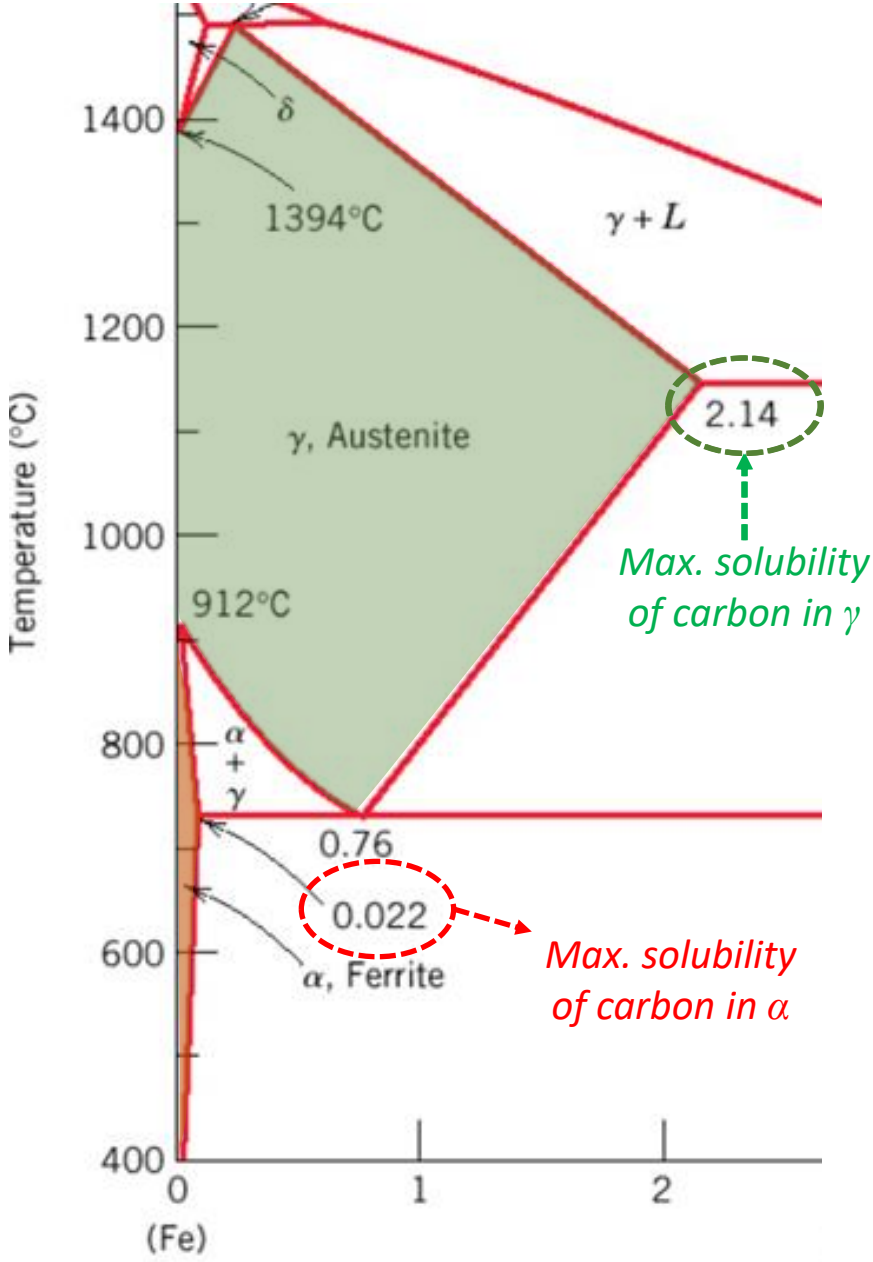
727 °C, 0.76 wt.% C

- Why the solubility of ‘Carbon’ is more in the austenite phase (FCC) than in ferrite (BCC)??
- How does a carbon atom dissolve in an iron matrix?

- Carbon occupies the ***interstitial sites*** in an iron crystal structure.

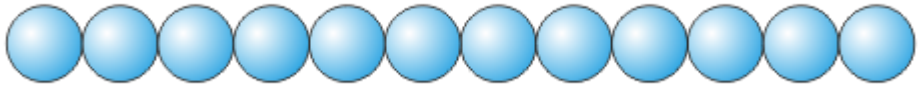
  Atomic radius of a carbon atom = 70 pm

- Volume fraction of BCC = 68%
- Volume fraction of FCC = 74%
- Empty space is higher in BCC.

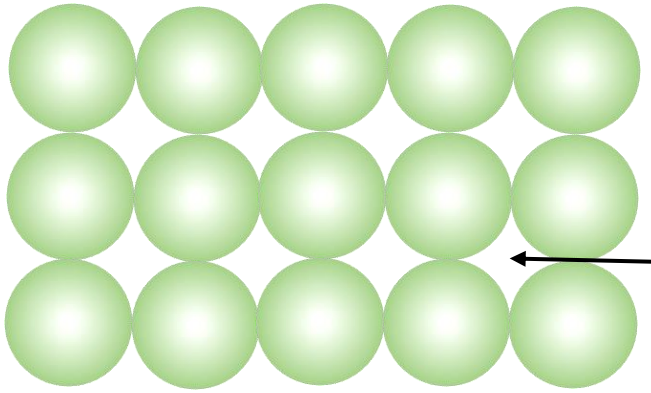


Packing sequence in cubic lattices

- **Close-packing in 1-D**

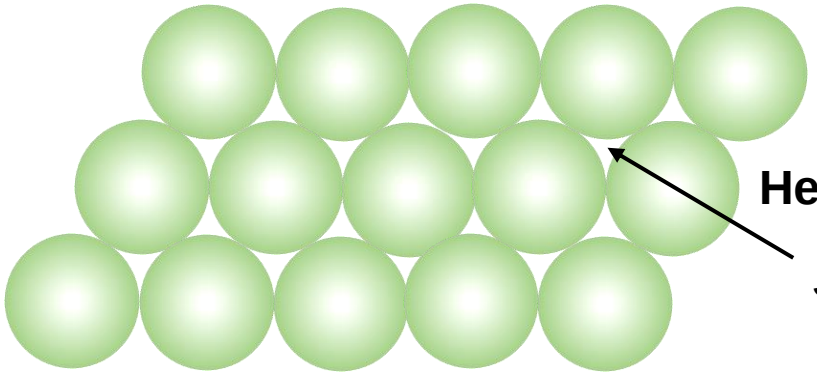


- **Close-packing in 2-D**



Square (primitive) packing

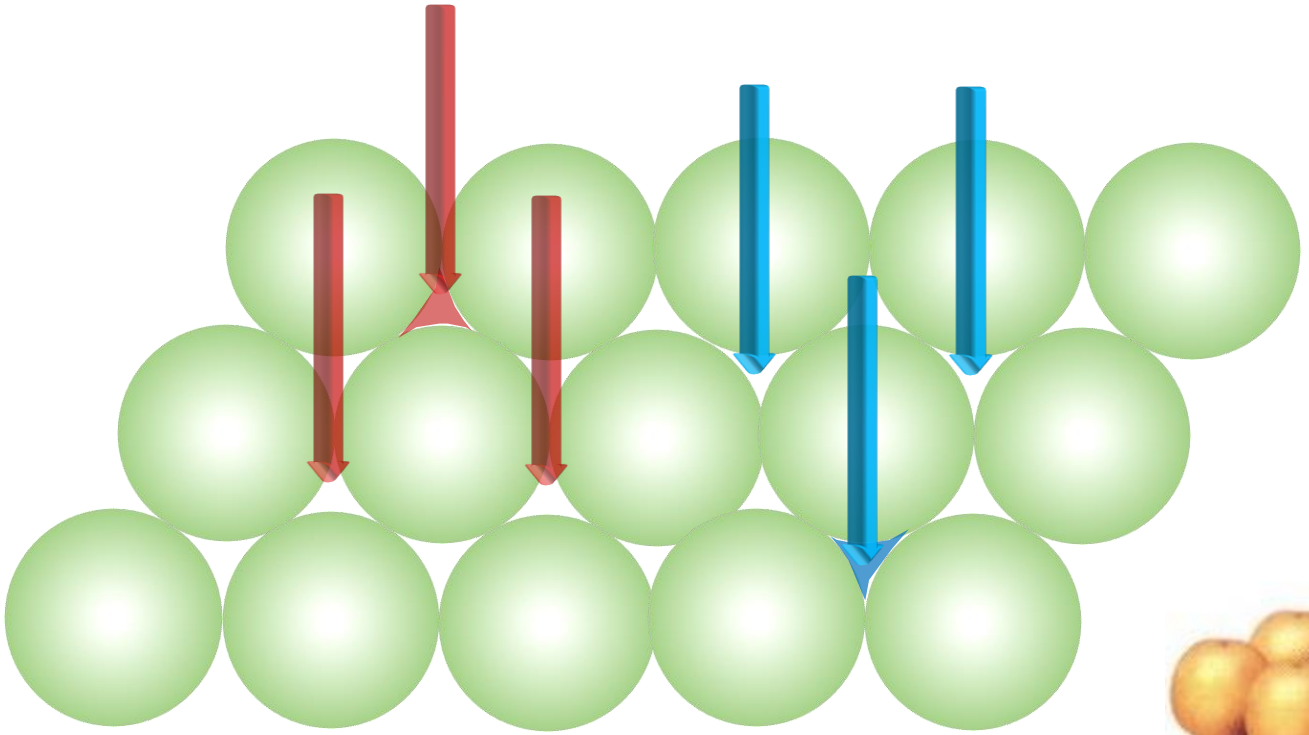
Large voids, low space-filling

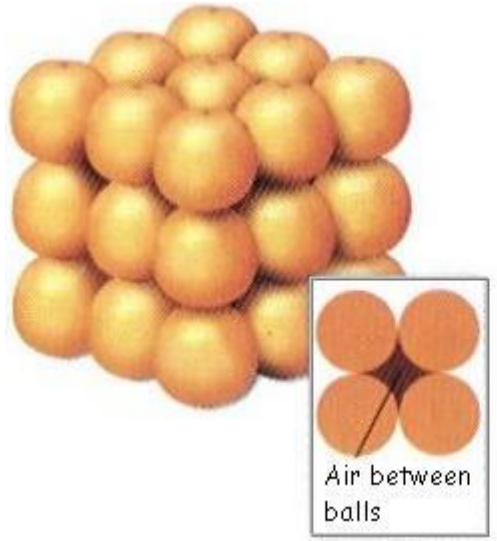


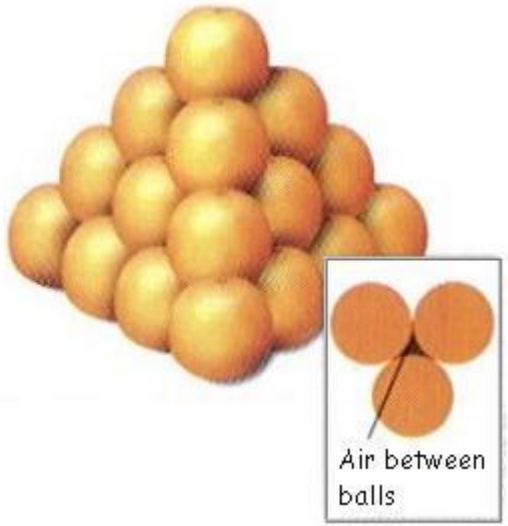
Hexagonal close packing

Small voids, high space-filling

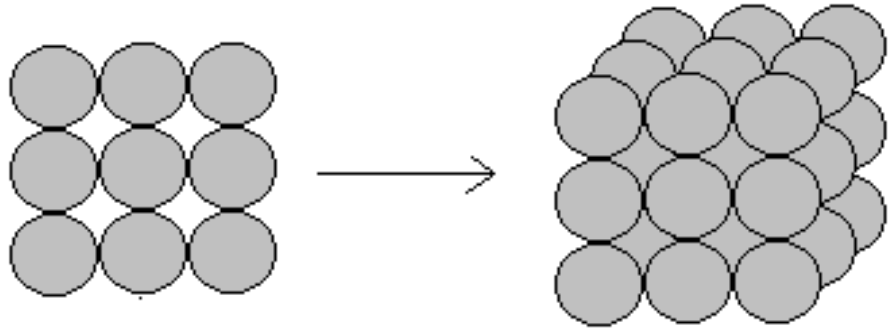
- **Close-packing in 3-D ??**



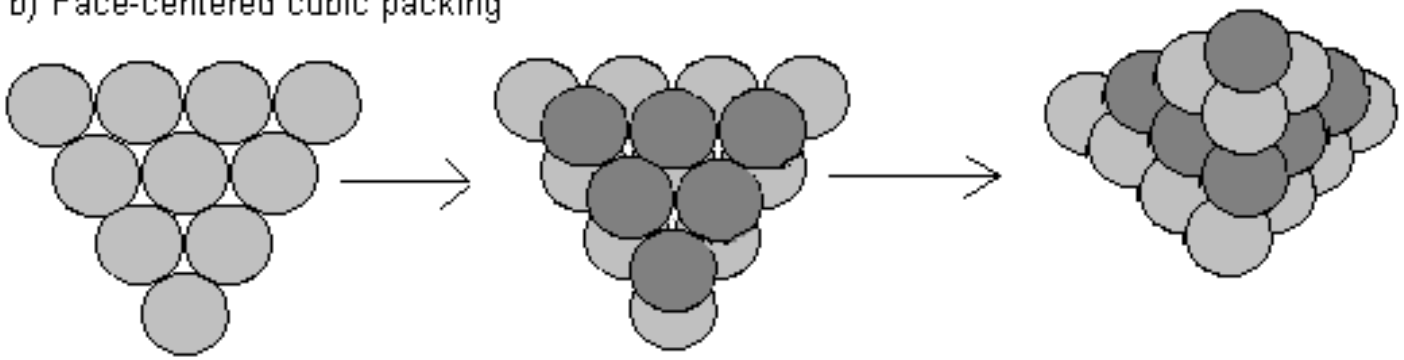




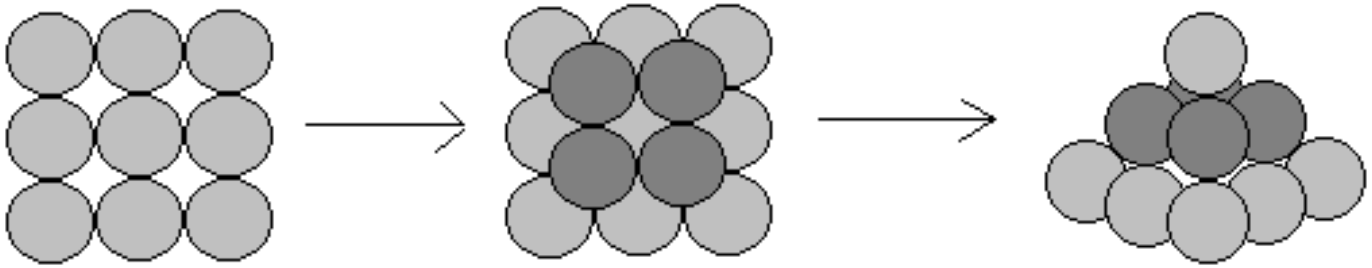
a) Simple cubic packing

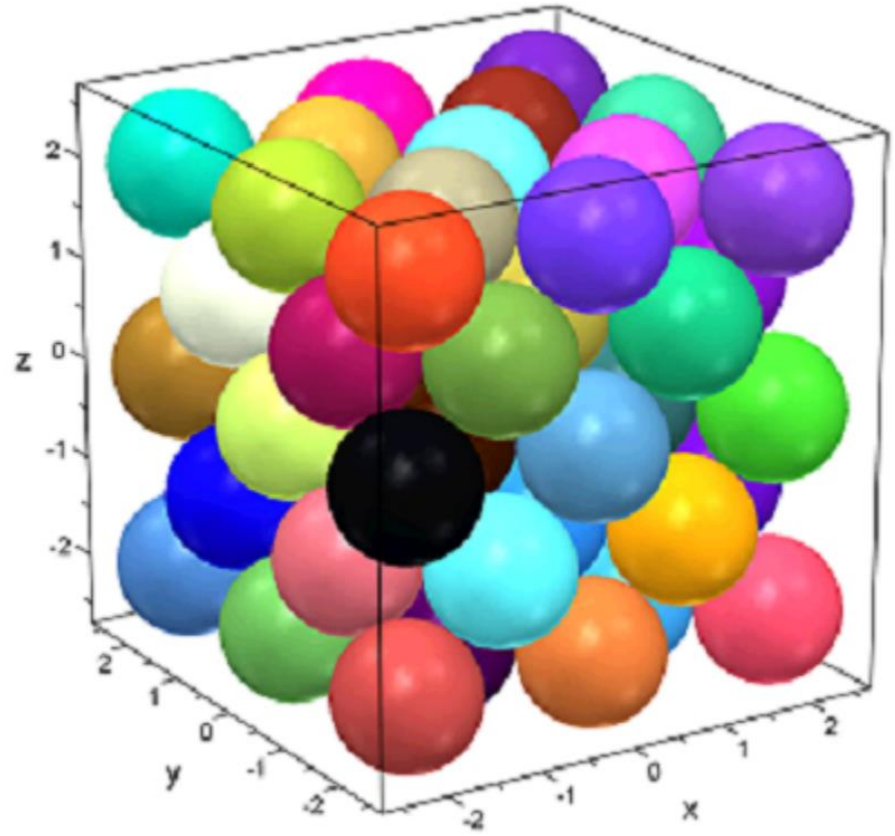


b) Face-centered cubic packing

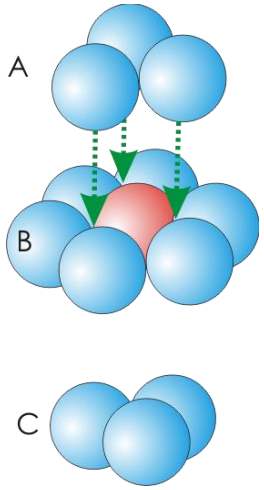


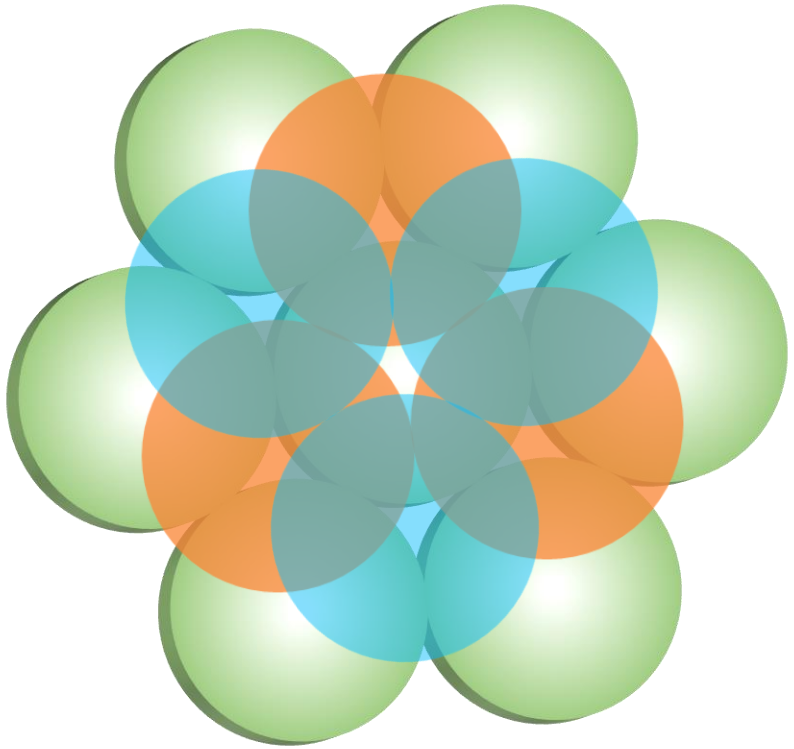
c) Hexagonal packing

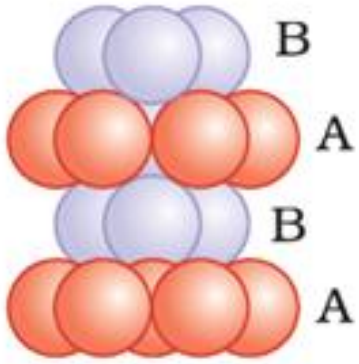


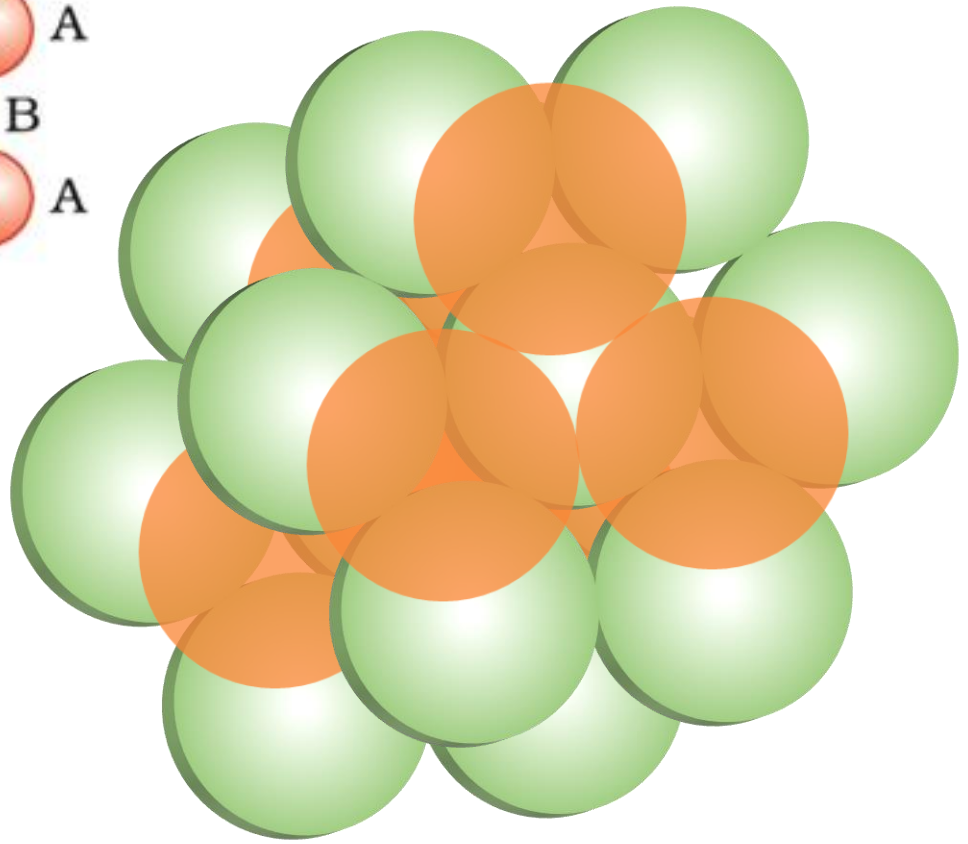


Close-packing in 3-D



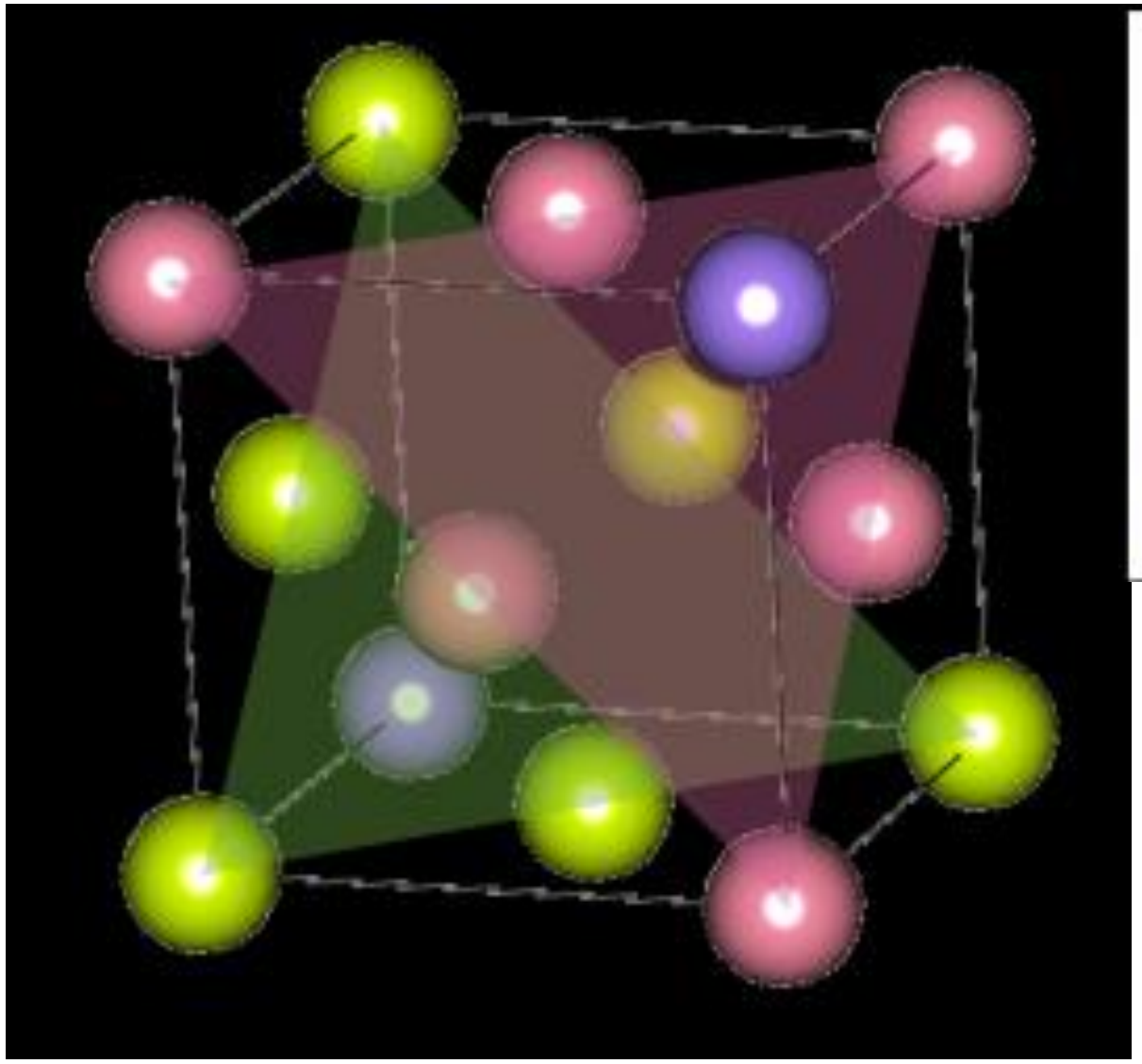


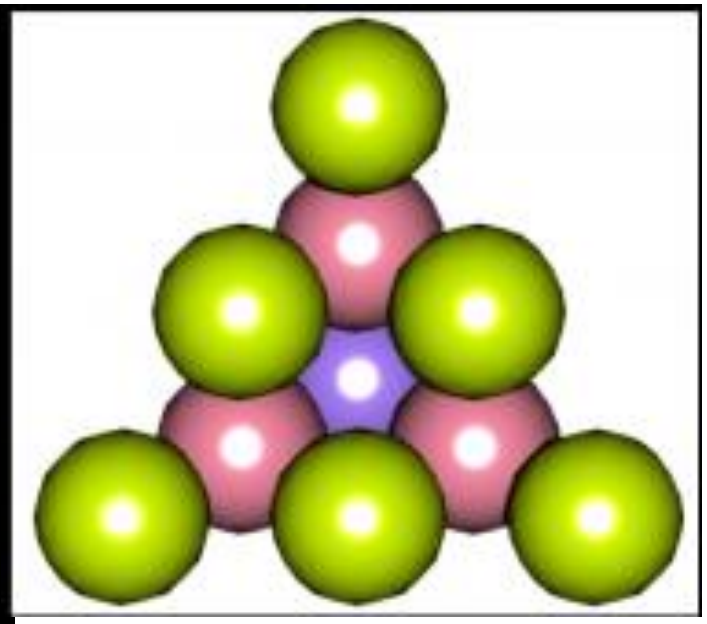




Stacking sequence	ABCABC…..	ABAB…..
Close packing type	Cubic close packing (CCP)	Hexagonal close packing (HCP)

Face-centred cubic

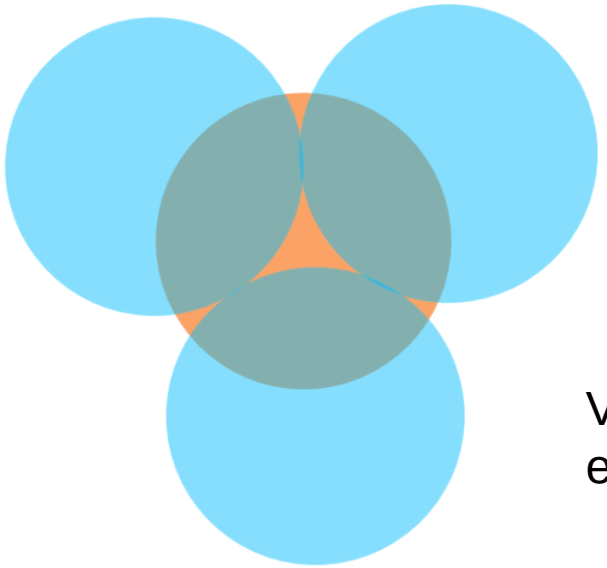


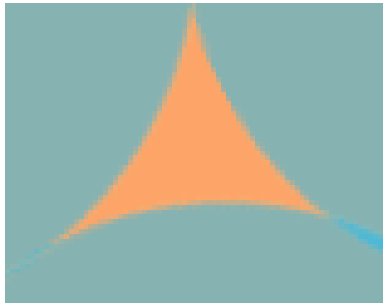


- Close-packed plane in FCC: {111}
- Close-packed direction in FCC: <110>

Empty spaces enclosed by atoms in a crystal: Voids

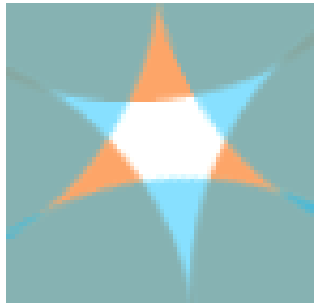
Voids in close-packed structures





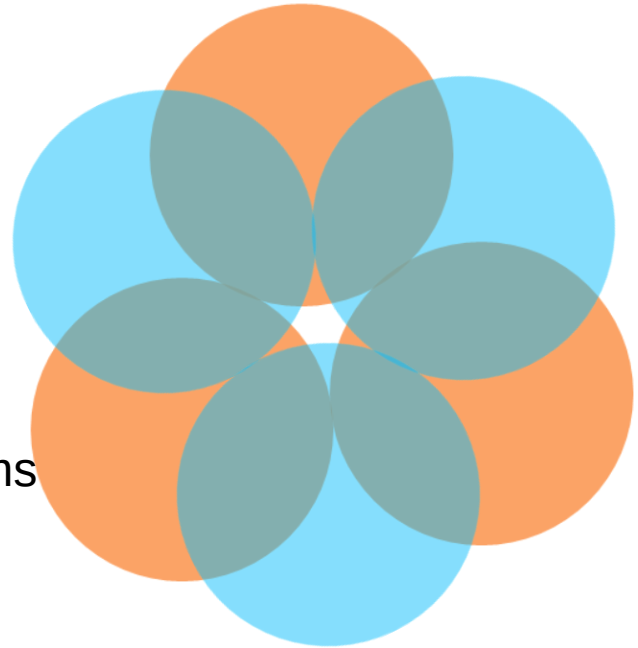
Tetrahedral void
(TV)

Void forms with 4 atoms enclosing the space



Octahedral void
(OV)

Void forms with 6 atoms enclosing the space



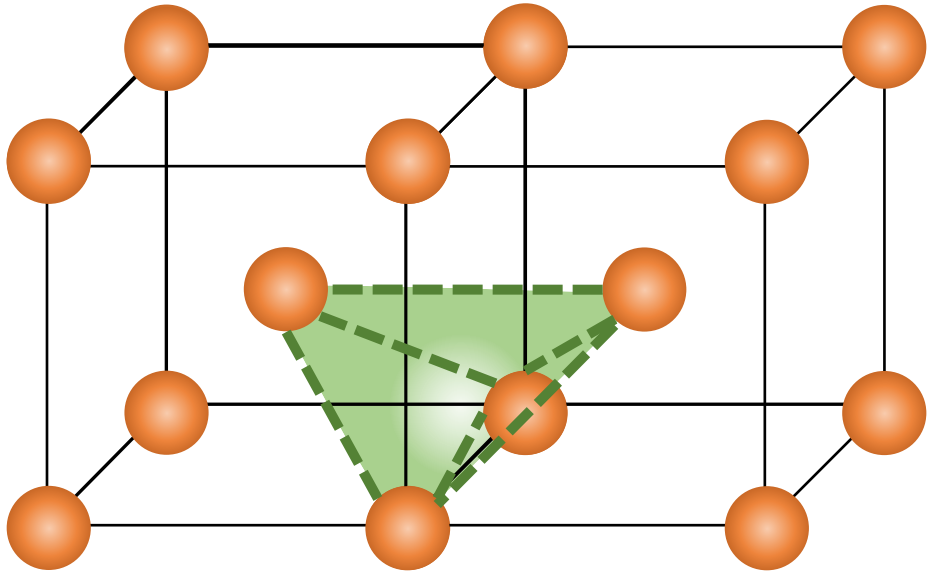
Co-ordination number

4

6

How many tetrahedral and octahedral voids are present in ferrite (BCC) and austenite (FCC)?

Tetrahedral voids in BCC



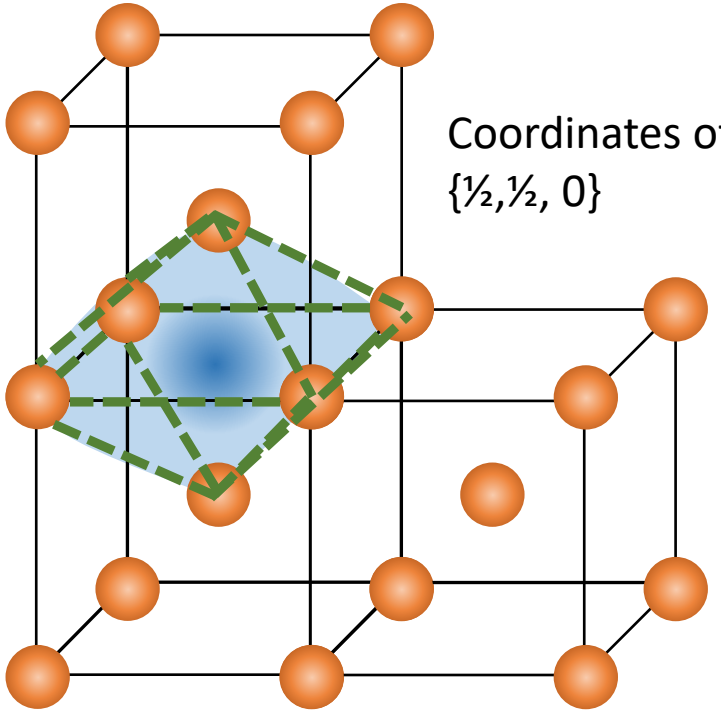
Coordinates of the void:
{½, 0, ¼} *(four on each face)*

- No. of faces: 6

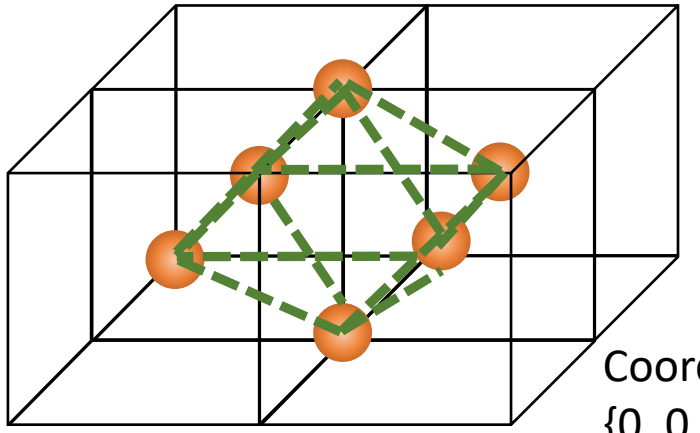
- Total no. of ‘T’ voids: 24
- No. of ‘T’ voids per unit cell : (24/2) = 12

- No. of ‘T’ voids per unit atom: (12/2) = 6

Octahedral voids in BCC

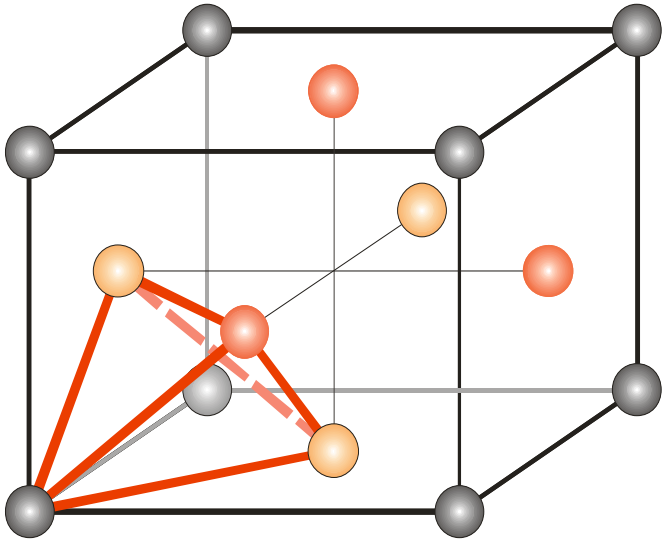


Coordinates of the void:
{½,½, 0}

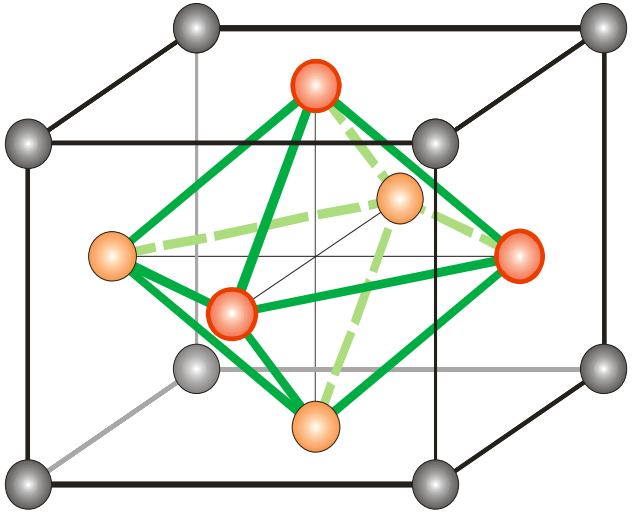


Coordinates of the void:
{0, 0, ½}

Tetrahedral voids in FCC



Octahedral voids in FCC



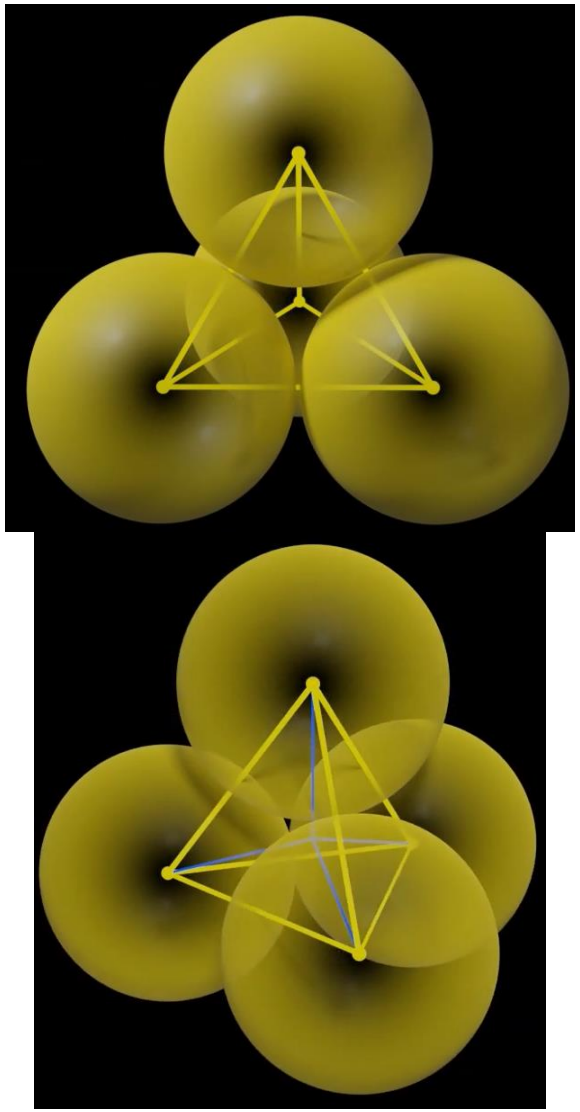
Number of voids in BCC and FCC

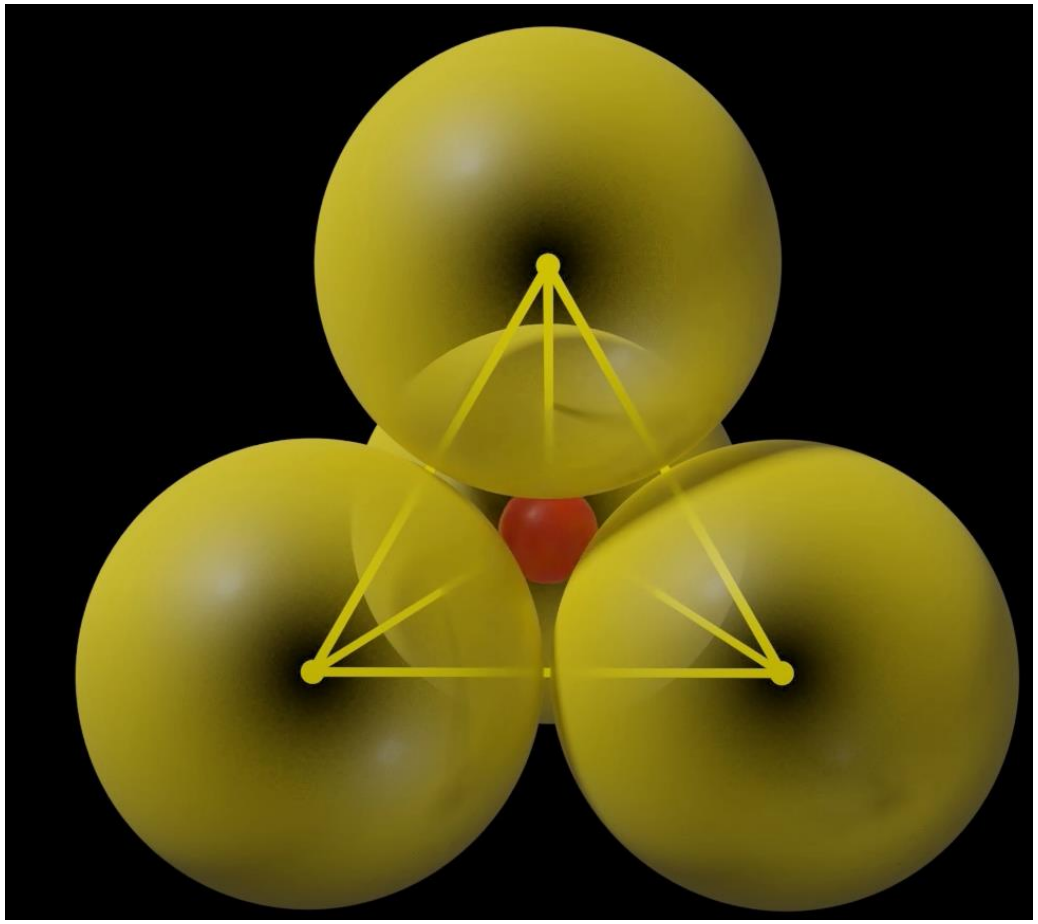
BCC voids	Position	Voids / cell	Voids / atom
Distorted Tetrahedral	• Four on each face: [(4/2) × 6 = 12] → (0, ½, ¼)	12	6
Distorted Octahedral	• Face center: (6/2 = 3) → (½, ½, 0) • Edge center: (12/4 = 3) → (½, 0, 0)	6	3

FCC voids	Position	Voids / cell	Voids / atom
Tetrahedral	¼ way from each vertex of the cube along body diagonal <111> → ((¼, ¼, ¼))	8	2
Octahedral	• Body centre: 1 → (½, ½, ½) • Edge centre: (12/4 = 3) → (½, 0, 0)	4	1

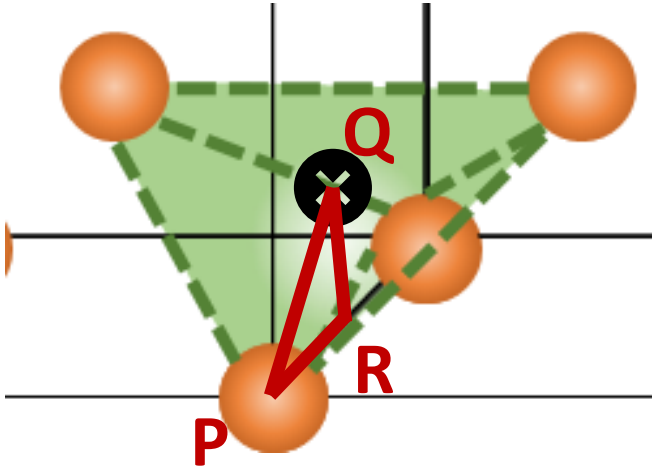
- ❑ Number of 'T' voids is greater than those of 'O' voids.
- ❑ But, still Carbon prefers to occupy the 'O' voids.

What is the size of the largest atom which can fit into a tetrahedral void of BCC?





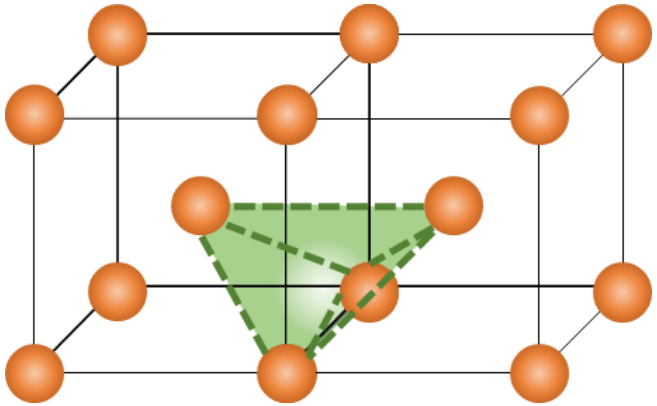
What is the size of the largest atom which can fit into a tetrahedral void of BCC?



Consider ΔPQR,

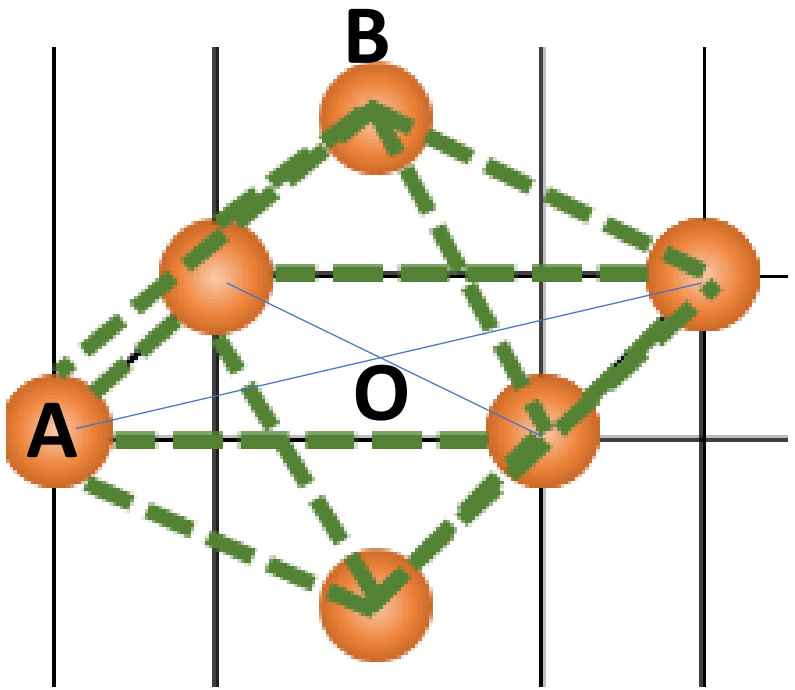
$$PQ = \sqrt{\frac{a^2}{(4)^2} + \left(\frac{a^2}{4}\right)} = (r + x) = \frac{\sqrt{5}}{4}.a$$

In a BCC crystal system, $a = \frac{4.r}{\sqrt{3}}$

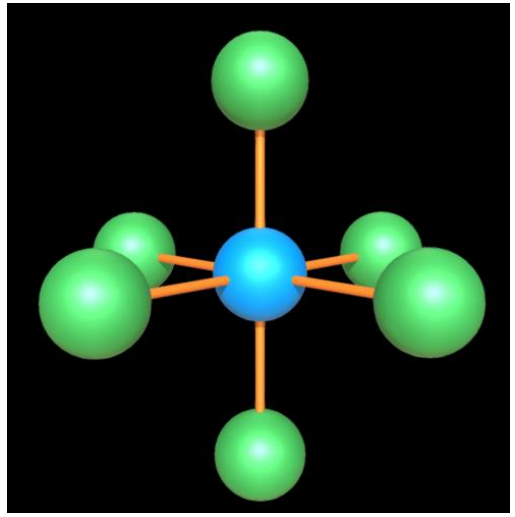


$$x = 0.29.r$$

What is the size of the largest atom which can fit into a octahedral void of BCC?



- Distance (OA) = $\frac{a}{\sqrt{2}}$ = 0.707 a
- Distance (OB) = $(\frac{a}{2})$ = 0.5 a
- Since the length of OB is smaller than OA, the atom situated at the Octahedral void is expected to touch the body-centred atom (point 'B').



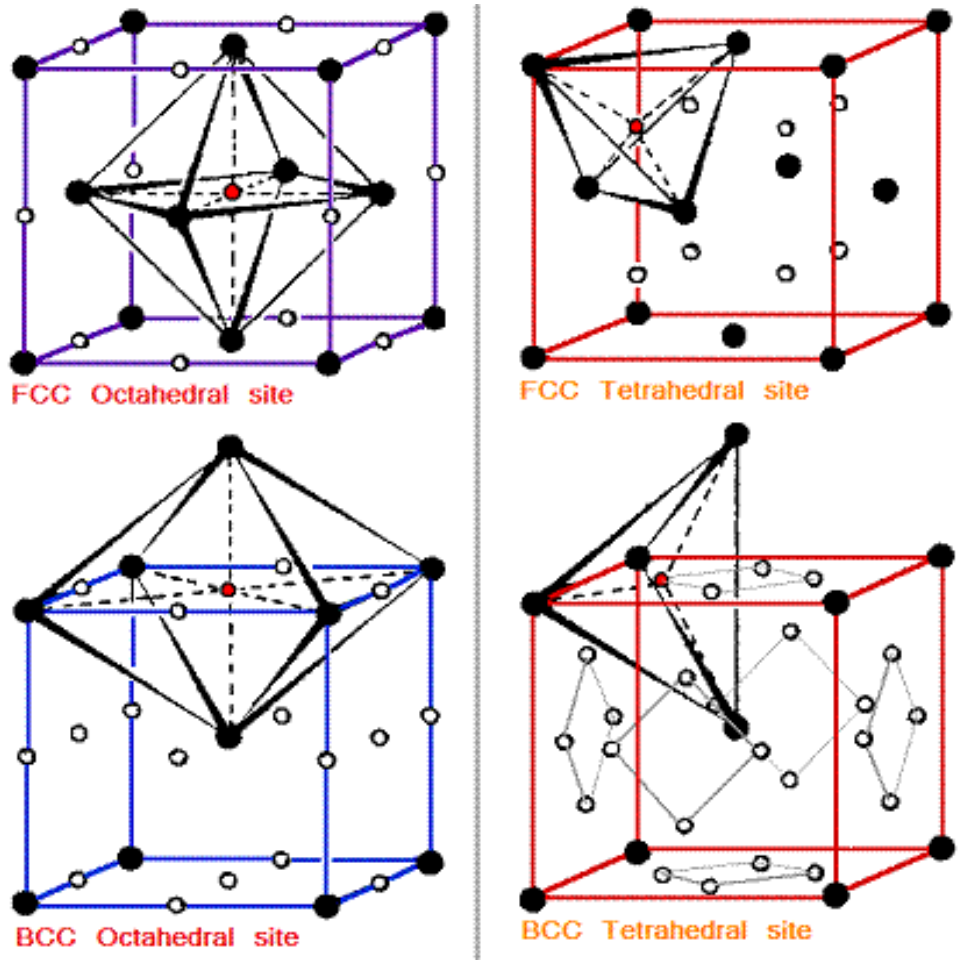
$$OB = r + x = \frac{a}{2}$$

$$r + x = \frac{4r}{2\sqrt{3}} \qquad BCC: \sqrt{3}a = 4r$$

$$\frac{x}{r} = \left(\frac{2\sqrt{3}}{3} - 1\right) = 0.1547$$

BCC voids	Position	Voids / cell	Voids / atom
Distorted Tetrahedral	• Four on each face: [(4/2) × 6 = 12] → (0, ½, ¼)	12	6
Distorted Octahedral	• Face center: (6/2 = 3) → (½, ½, 0) • Edge center: (12/4 = 3) → (½, 0, 0)	6	3

	BCC	FCC
Octahedral	0.155 *(distorted)*	0.414
Tetrahedral	0.29 *(distorted)*	0.225



➢ ***Why interstitial atoms prefer to occupy the octahedral positions?***