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Seven Primitive Unit cells and their Possible Variations as Centered Unit Cells

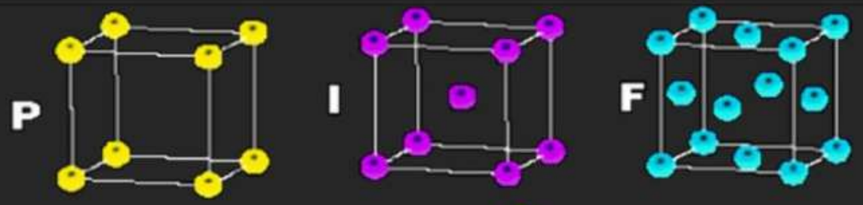
Crystal system	Possible Variations (Unit cell)	Axial distance or edge lengths	Axial angles	Examples
Cubic	Primitive Body centered Face centred	a = b = c	$\alpha = \beta = \gamma = 90^\circ$	NaCl, Zinc blende, Cu
Tetragonal	Primitive Body centered.	a = b ≠ c	$\alpha = \beta = \gamma = 90^\circ$	White tin, SnO_2, TiO_2, $CaSO_4$
Orthorhombic	Primitive Body centered. Face centered, End centered	a ≠ b ≠ c	$\alpha = \beta = \gamma = 90^\circ$	Rhombic sulphur, KNO_3, $BaSO_4$
Hexagonal	Primitive	a = b ≠ c	$\alpha = \beta = 90^\circ$ $\gamma = 120^\circ$	Graphite, ZnO CdS
Rhombohedral or Trigonal	Primitive	a = b = c	$\alpha = \beta = \gamma \neq 90^\circ$	Calcite ($CaCO_3$), HgS (Cinnabar)
Monoclinic	Primitive End centred	a ≠ b ≠ c	$\alpha = \gamma = 90^\circ$ $\beta \neq 90^\circ$	Monoclinic suphur $Na_2, SO_4, 10H_2O$
Triclinic	Primitive	a ≠ b ≠ c	$\alpha \neq \beta \neq \gamma \neq 90^\circ$	K_2CrO_7, $CuSO_4.5H_2O$, H_3O

(Bravais lattices)
14 Unit cell
repeat
lattice
Basis
Crystal

CUBIC

$a = b = c$

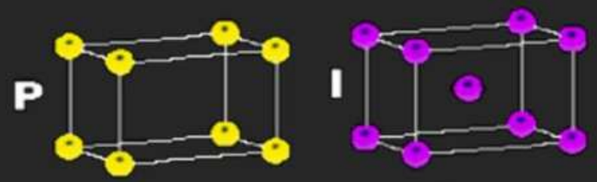
$\alpha = \beta = \gamma = 90°$



TETRAGONAL

$a = b \neq c$

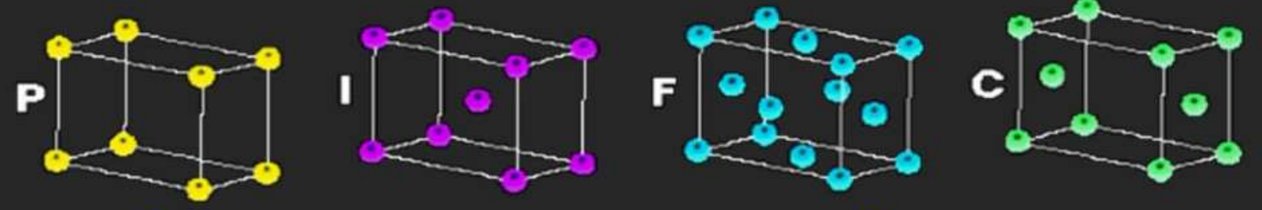
$\alpha = \beta = \gamma = 90°$



ORTHORHOMBIC

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$



HEXAGONAL

$a = b \neq c$

$\alpha = \beta = 90°$

$\gamma = 120°$

TRIGONAL

$a = b = c$

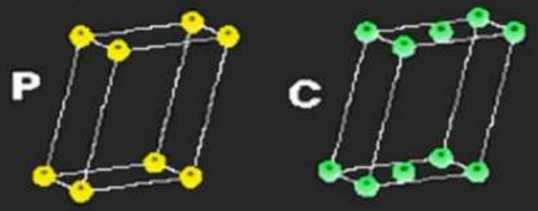
$\alpha = \beta = \gamma \neq 90°$

MONOCLINIC

$a \neq b \neq c$

$\alpha = \gamma = 90°$

$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$

$\alpha \neq \beta \neq \gamma \neq 90°$

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ **14 Bravais Lattices**

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Arrangement of identical atoms.

(1) In 1-D

(2) In 2-D

(1) 2-D Square close packing

(2) 2-D hexagonal close packing

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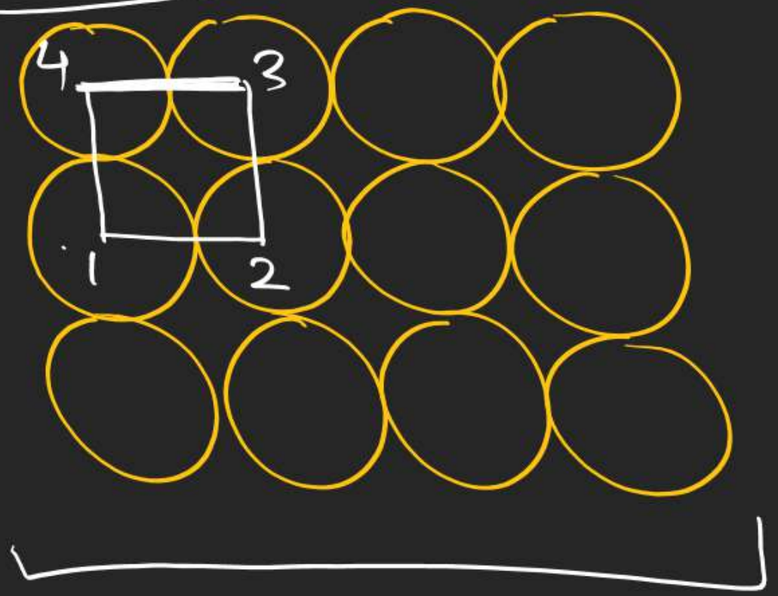
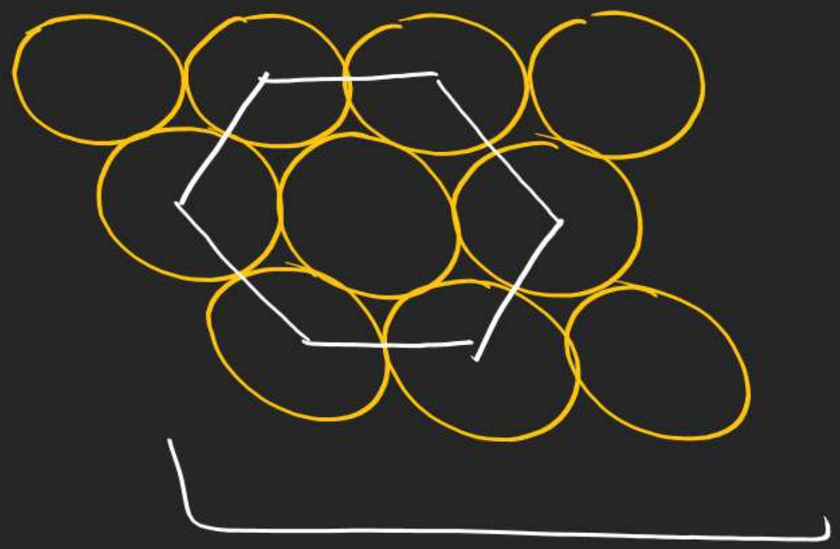
Square



P Body

hexagonal close



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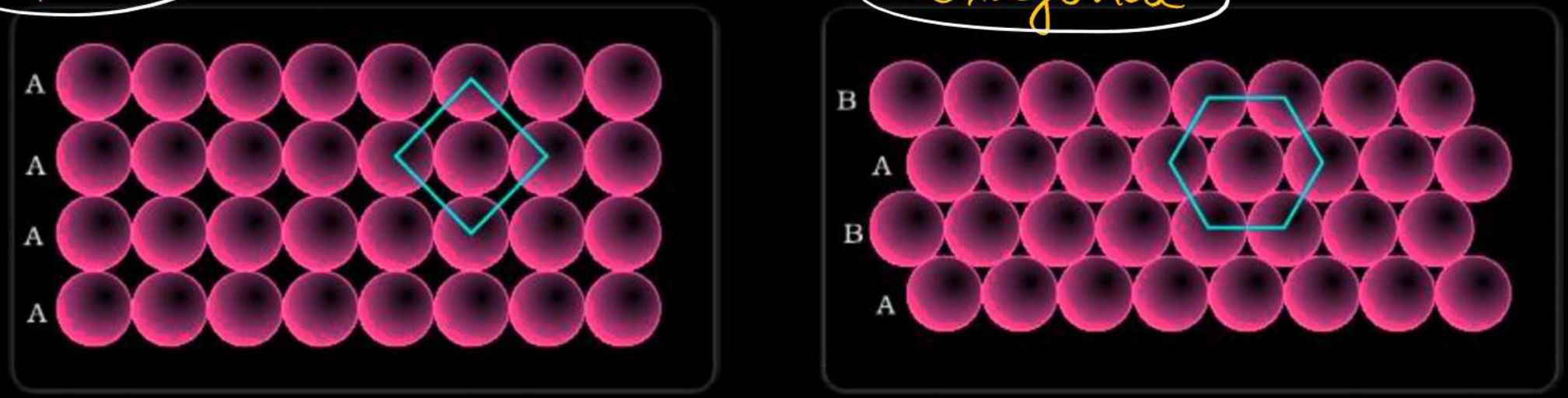
1-D

Close packing of spheres in one dimension

Square

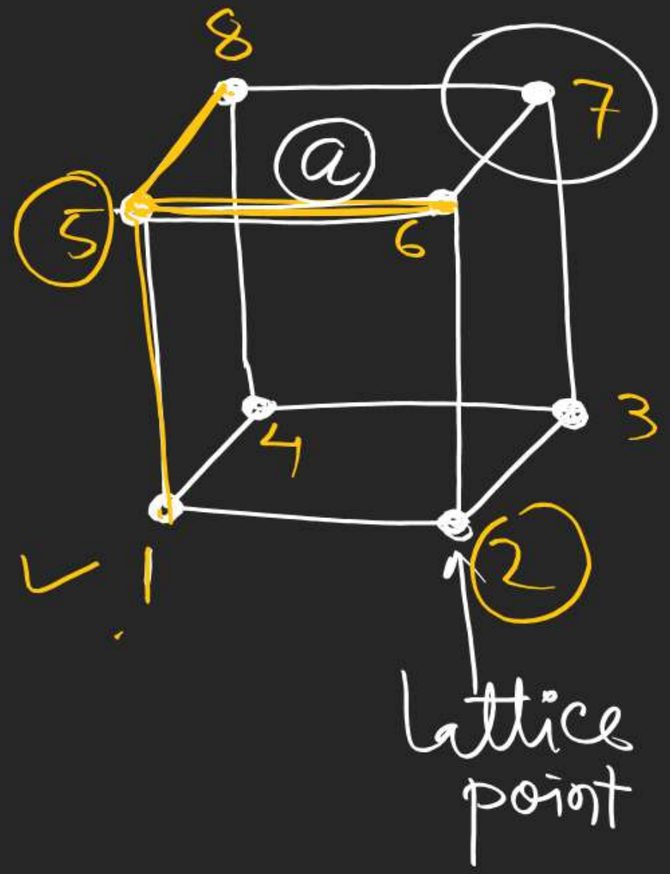
hexagonal



(a) (b)

(a) Square close packing (b) hexagonal close packing of spheres in two dimensions

Primitive Cubic unit cell (Simple cubic unit cell)

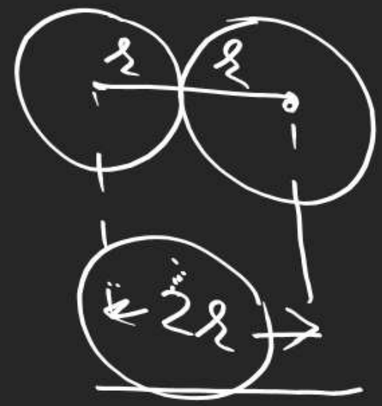


2 ⟶ 1, 3, 6

5 ⟶ 1, 6, 8

(1) Atoms at the adjacent corner touch each other

(2) $a = 2r$



(3) No. of atoms per unit cell in simple cube $= \frac{1}{8} \times 8 = 1$

(4) Co-ordination no.: No. of atoms in direct contact with a given atom

$= 6$

(5) Packing effeciency $\Rightarrow$ Volume of cube $= a^3$

Volume of an atom $= \frac{4}{3}\pi r^3$

$$\text{Packing efficiency} = \frac{1 \times \frac{4}{3}\pi r^3}{a^3} \times 100$$

$(a = 2r)$

$$= 52.4\%$$

→ distance of nearest atom from a given atom and no. of such atoms? a / 6

→ distance of 2nd nearest atom ? $\sqrt{2}a$ / 12

→ Third nearest ?

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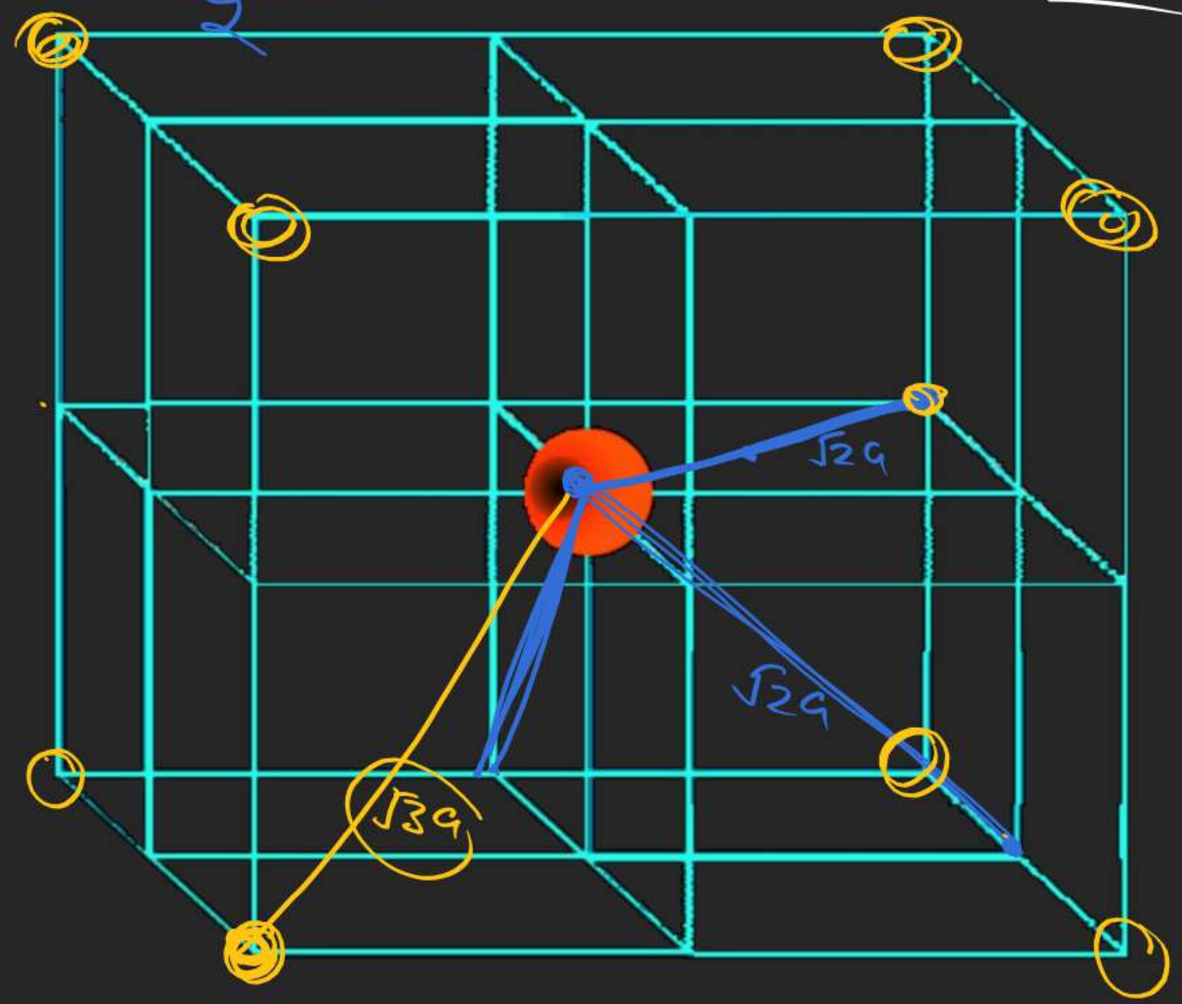
$\sqrt{2}a$

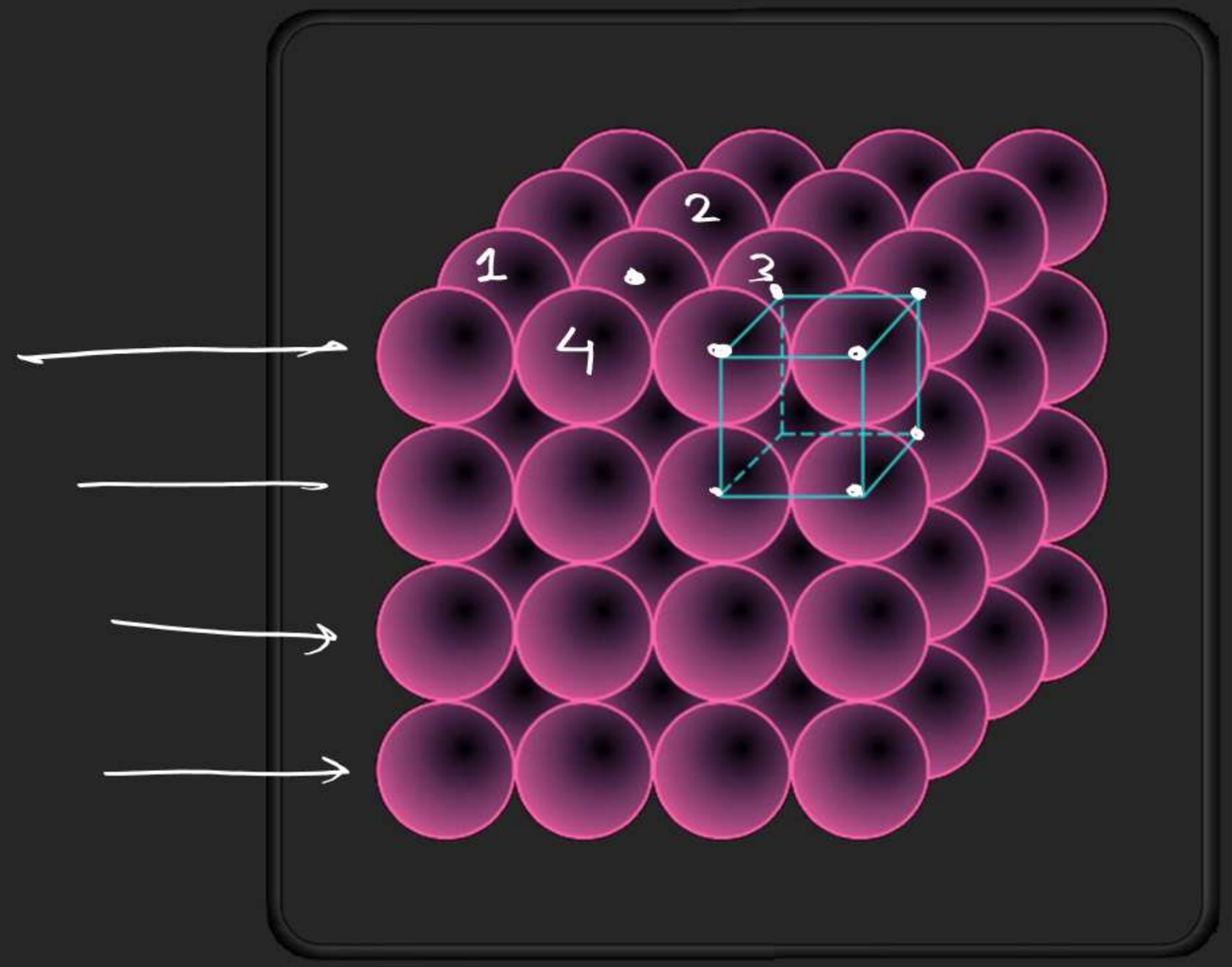
$$12 = \frac{8 \times 3 = 24}{2} \quad \text{—(3)}$$



$\frac{1}{8}^{th}$ Corner

$\frac{1}{2}^{th}$ atom at the face centre

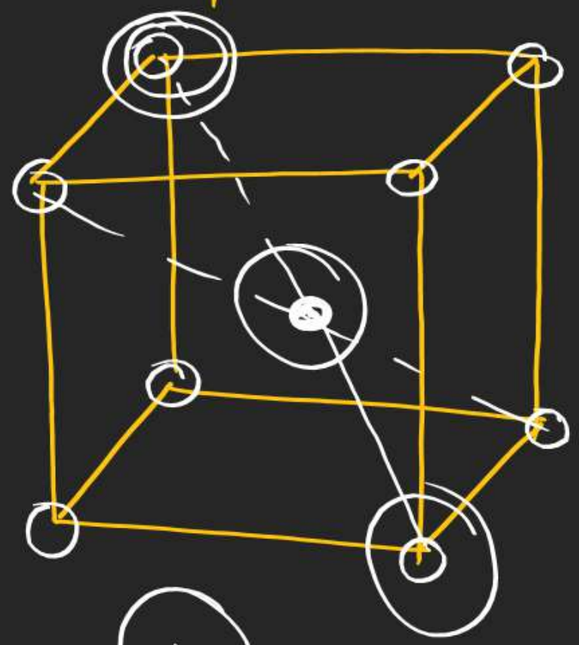
$\frac{1}{4}^{th}$ atom at the edge centre



6

Fig. 1.19: *Simple cubic lattice formed by A A A .... arrangement*

Body centred cubic unit cell

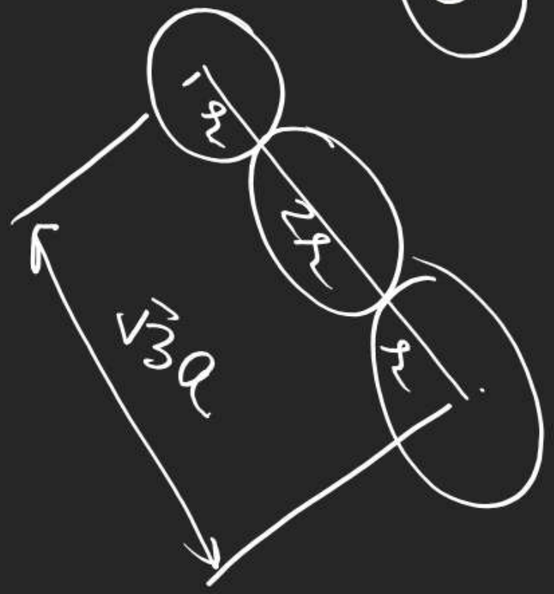


① atoms at the adjacent corner do not touch ~~other~~ each other

$(a > 2r)$

② atoms along the body diagonal touch each other

$\sqrt{3}a = 4r$



③ No of atoms per unit cell $= \frac{1}{8} \times 8 + 1$

$= 1 + 1$

$= 2$

④ Co-ordination no. = 8

⑤ Packing efficiency = ?

Sheet O-I 1-15

S-I 1-5

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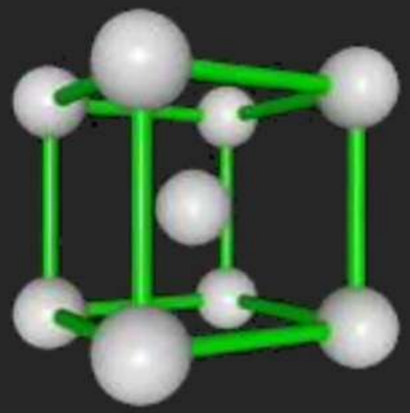

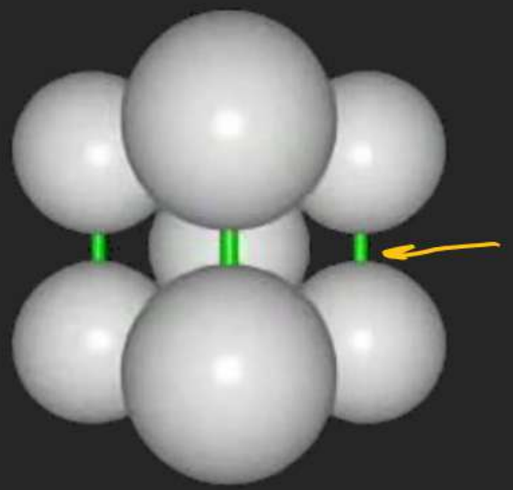

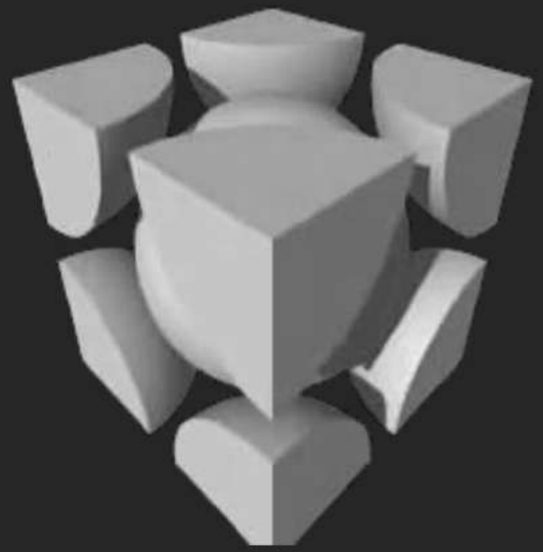

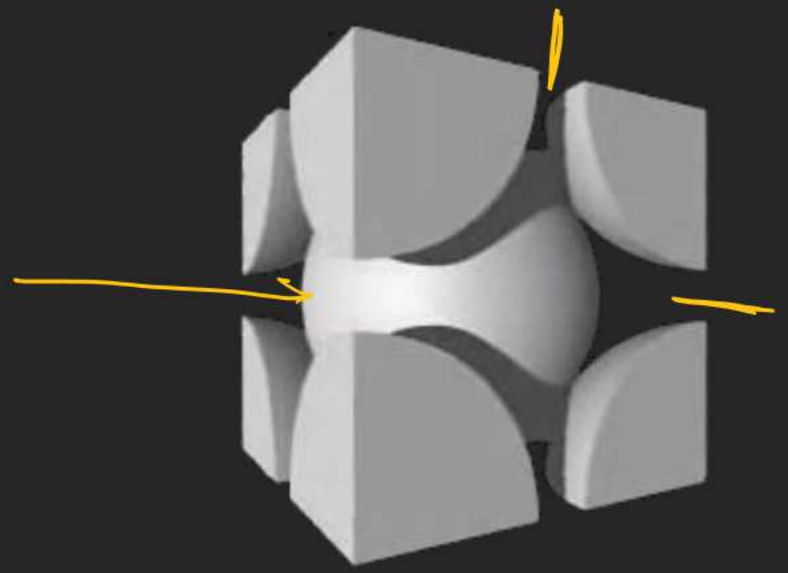

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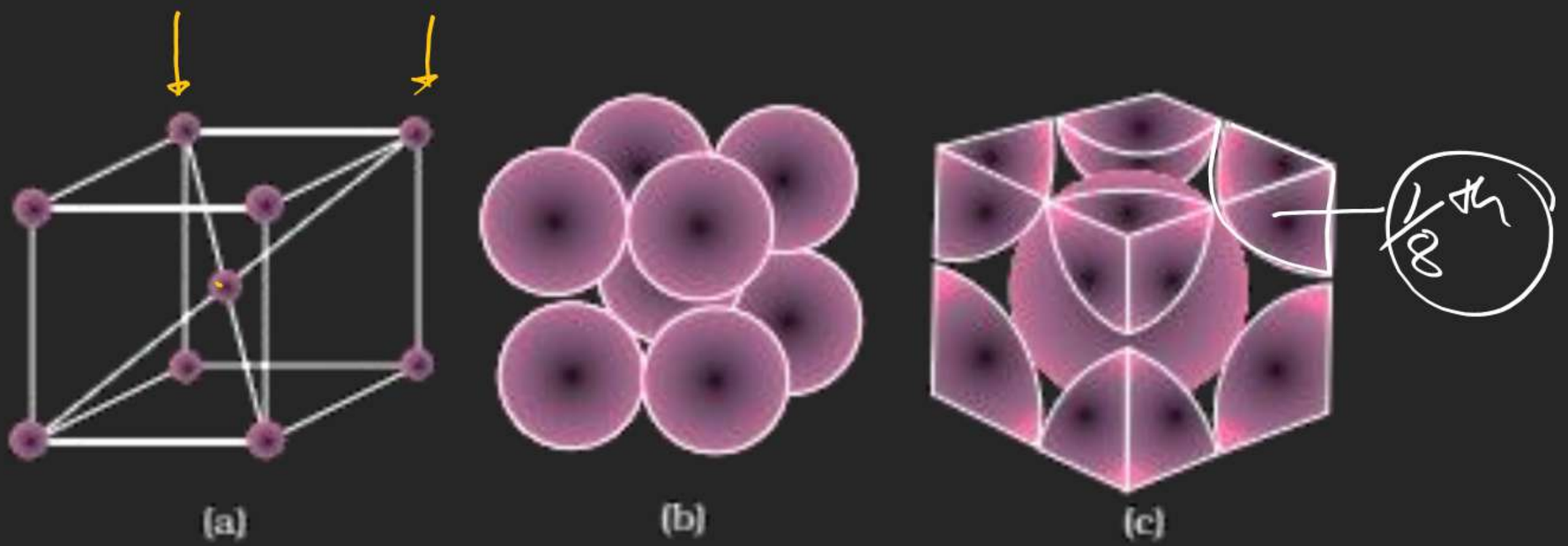
BCC



A primitive cubic unit cell (a) open structure (b) space-filling structure (c) actual portions of atoms belonging to one unit cell.

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