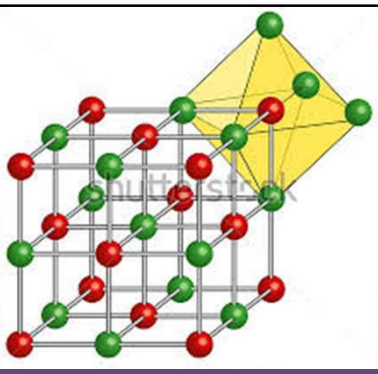


Structure of Solids

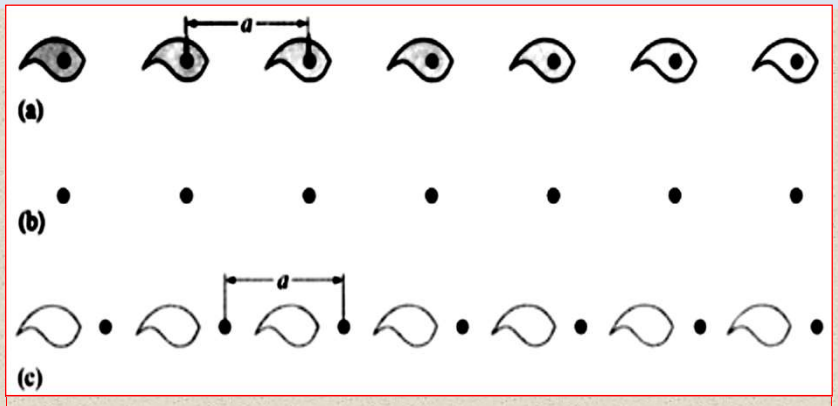
Prof Kamal M.S. Khalil

(2)

March 2020

أ.د/ كمال مُحَمَّد سيد خليل

1.6 LATTICES AND UNIT CELLS



A one-dimensional lattice (a, b) and the choice of unit cells (c)

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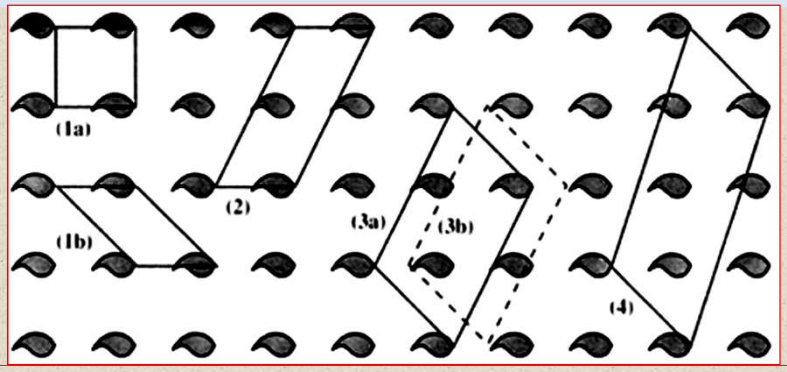
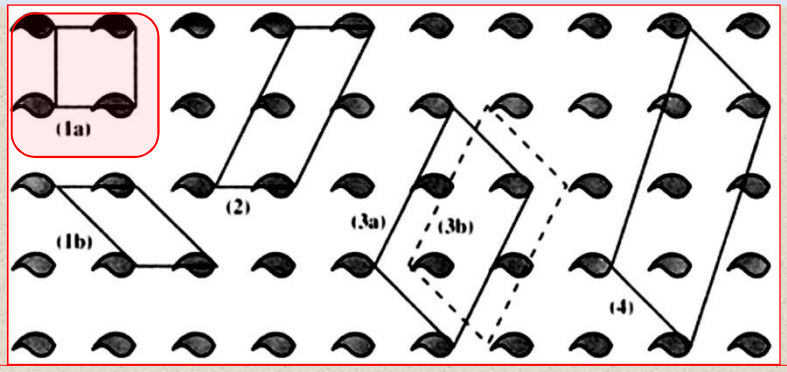
1.6 LATTICES AND UNIT CELLS



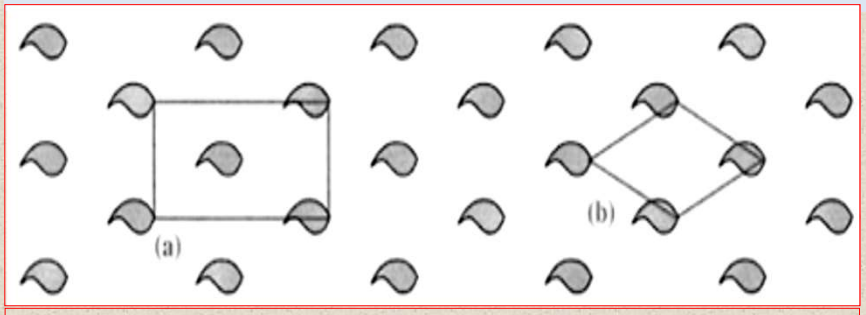
Choice of unit cell in a square two-dimensional lattice

1.6 LATTICES AND UNIT CELLS



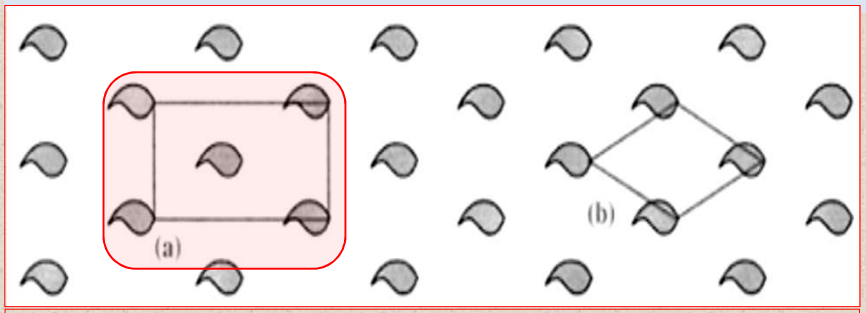
Choice of unit cell in a square two-dimensional lattice

1.6 LATTICES AND UNIT CELLS



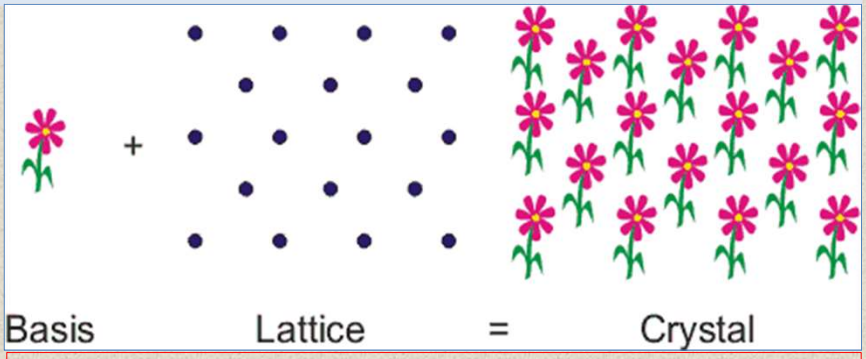
Choice of unit cell in a centred-rectangular lattice

1.6 LATTICES AND UNIT CELLS



Choice of unit cell in a centred-rectangular lattice

1.6 LATTICES AND UNIT CELLS



Draw a unit cell indicating the lattice vectors for the pattern of this crystal. What is the lattice type? How many atoms are there in the unit cell?

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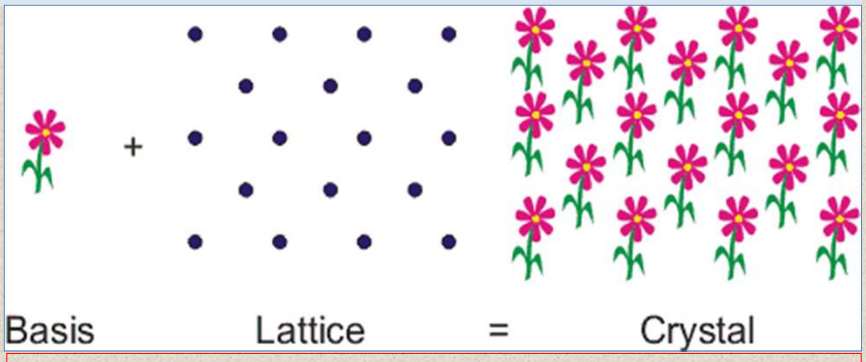
1.6 LATTICES AND UNIT CELLS



Draw a unit cell indicating the lattice vectors for the pattern of this crystal. What is the lattice type? How many atoms are there in the unit cell?

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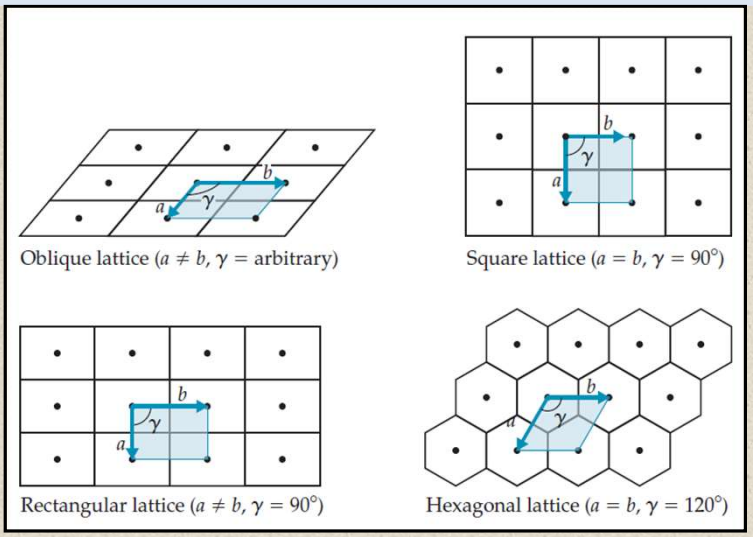
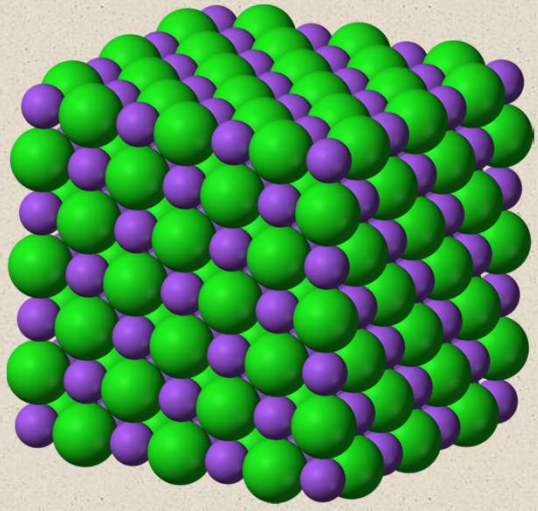
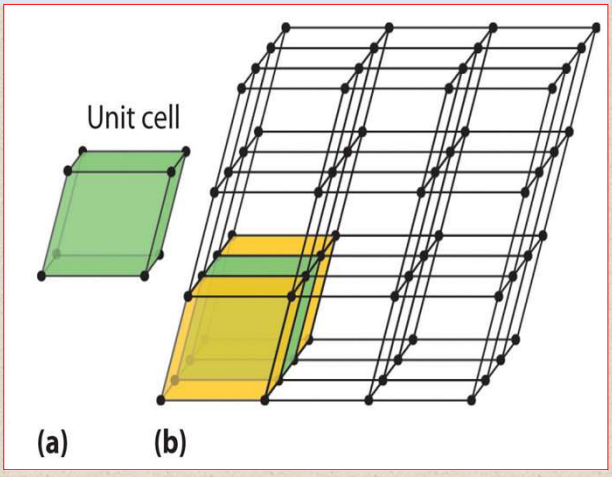
The four 2D lattices With Their UNIT CELLS



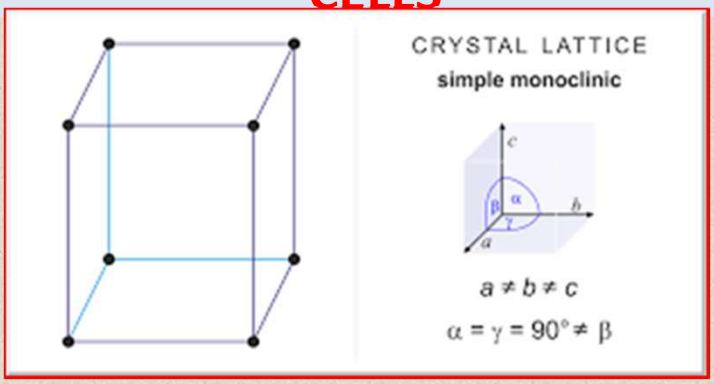
1.6.3 THREE-DIMENSIONAL UNIT CELLS



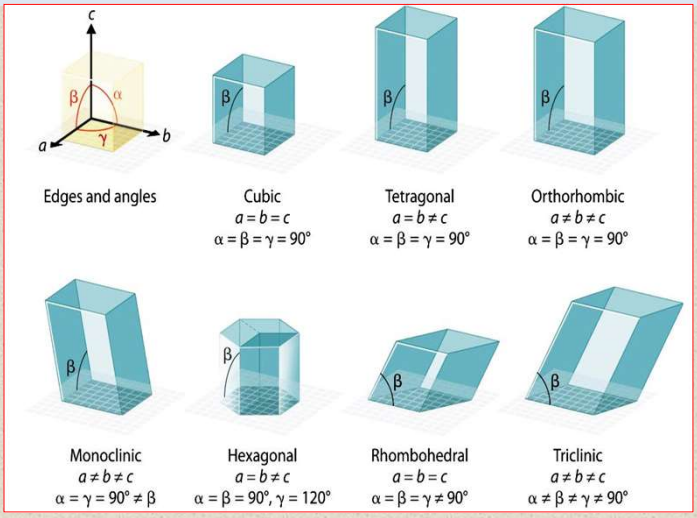
1.6.3 THREE-DIMENSIONAL UNIT CELLS



1.6.3 THREE-DIMENSIONAL UNIT CELLS



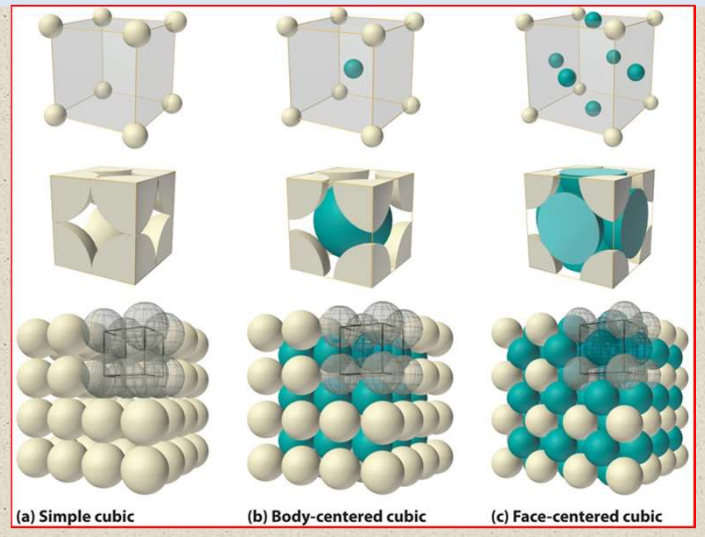
1.7 The Seven Basic Unit Cells



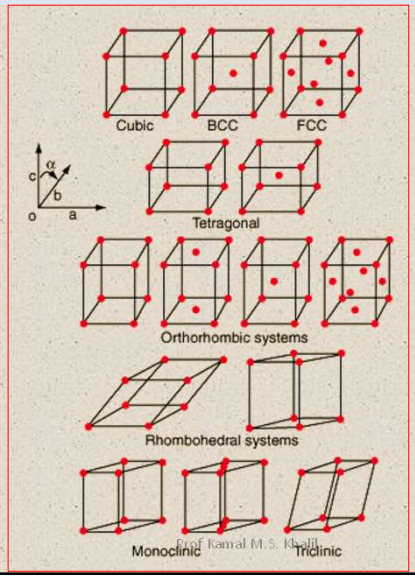
1.7 The Seven Basic Unit Cells

Crystal class	Axis system
Cubic	$a = b = c, \alpha = \beta = \gamma = 90^\circ$
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90^\circ$
Hexagonal	$a = b \neq c, \alpha = \beta = 90^\circ, \gamma = 120^\circ$
Rhombohedral	$a = b = c, \alpha = \beta = \gamma \neq 90^\circ$
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90^\circ$
Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90^\circ, \beta \neq 90^\circ$
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90^\circ$

Kinds of 3D Unit cells



1.8 The Fourteen Bravais Lattices.



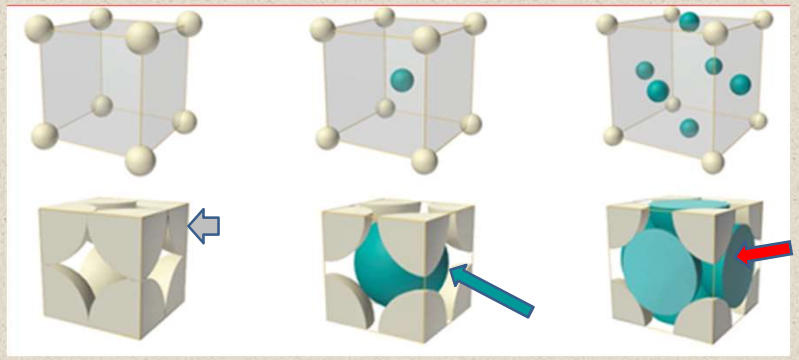
Density of solids

We need to know:

- The size of the unit cell (to obtain its volume),
- The molar mass of its components, and
- The number of components per unit cell.

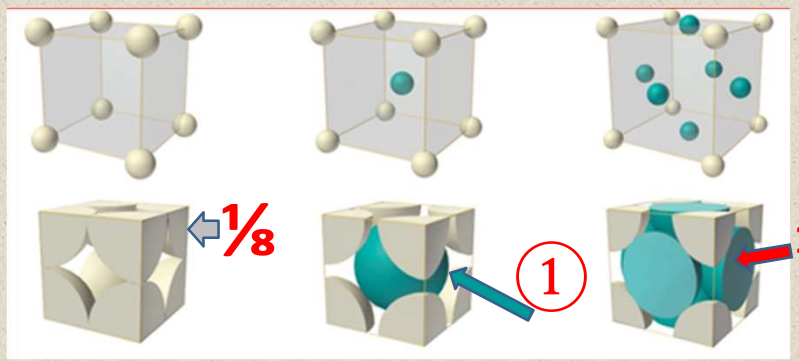
Density of solids

An atom that lies on a face, edge, corner or entirely within a unit cell.



Density of solids

An atom that lies on a face of a unit cell.
An atom that lies on the edge of a unit cell.
An atom at a corner of a unit cell.
Atoms that lie entirely within a unit celll.



Density of solids

Metallic gold has a face-centered cubic unit cell. How many Au atoms are in each unit cell?

Metallic has a body-centered cubic unit cell. How many Fe atoms are in each unit cell?

Density of solids

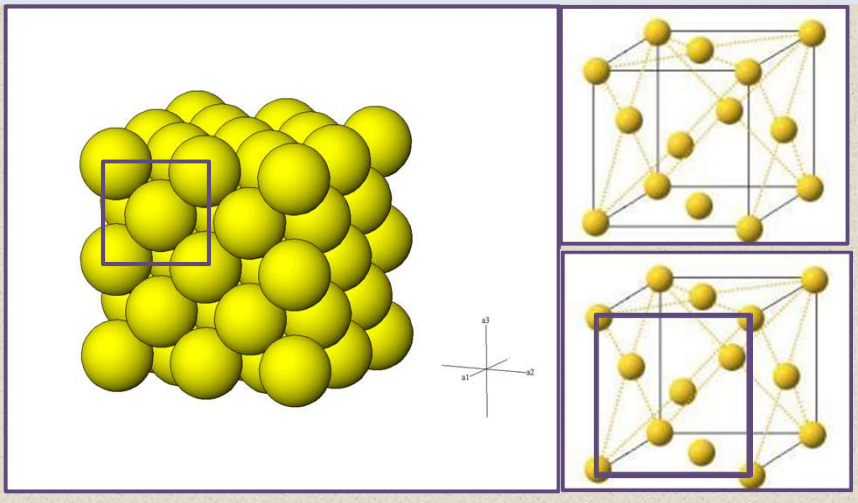
Calculate the density of metallic iron, which has a body-centered cubic unit cell with an edge length of 286.6 pm.

$$\text{mass of Fe} = (2 \cancel{\text{ atoms}}\ \text{Fe})\left(\frac{1\ \cancel{\text{mol}}}{6.022\times10^{23}\ \cancel{\text{atoms}}}\right)\left(\frac{55.85\ \text{g}}{\cancel{\text{mol}}}\right) = 1.855\times10^{-22}\ \text{g}$$

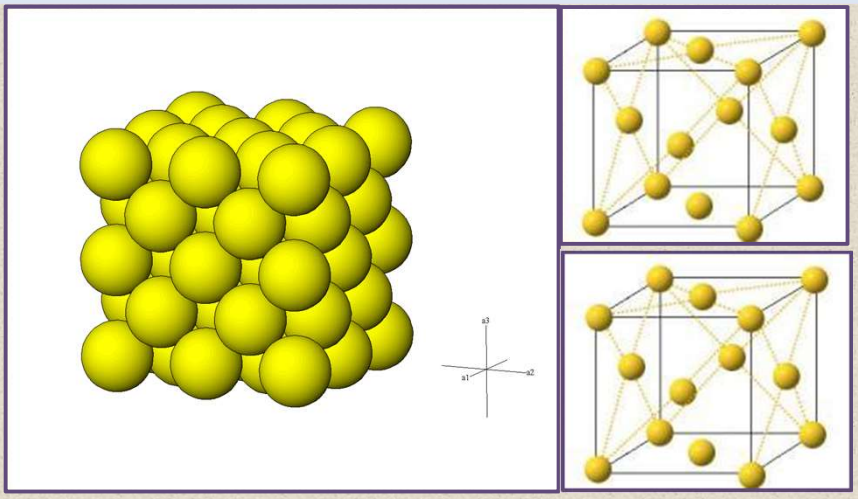
$$\text{volume} = \left[(286.6\ \cancel{\text{pm}})\left(\frac{10^{-12}\ \cancel{\text{m}}}{\cancel{\text{pm}}}\right)\left(\frac{10^{2}\ \text{cm}}{\cancel{\text{m}}}\right)\right]^{3} = 2.354\times10^{-23}\ \text{cm}^3$$

$$\text{density} = \frac{1.855\times10^{-22}\ \text{g}}{2.354\times10^{-23}\ \text{cm}^3} = 7.880\ \text{g/cm}^3$$

Density of solids



Density of solids



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Density of solids

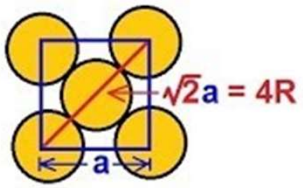
Face Centered Cube

Gold: Au

$\rho_{Au} = ?$

$R_{Au} = 144pm$

$Au_{Atomic\ Mass} = 197amu$



$\rho_{Au} = \frac{m}{V} = \frac{m}{a^3}$

$= \frac{(4atoms)(197amu/atoms)}{\left(\frac{4R}{\sqrt{2}}\right)^3}$

# of atoms = $8(\frac{1}{8}) + 6(\frac{1}{2})$

= 4 atoms

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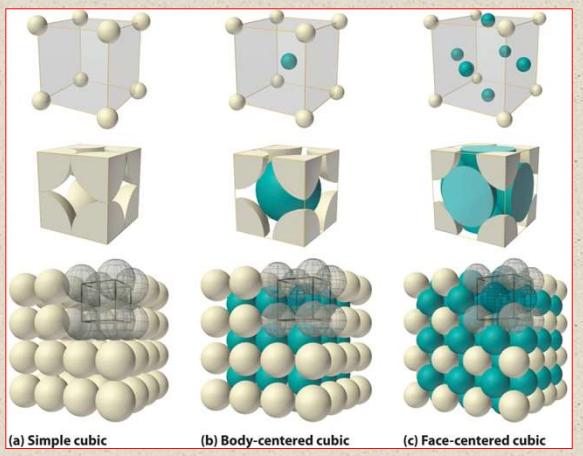
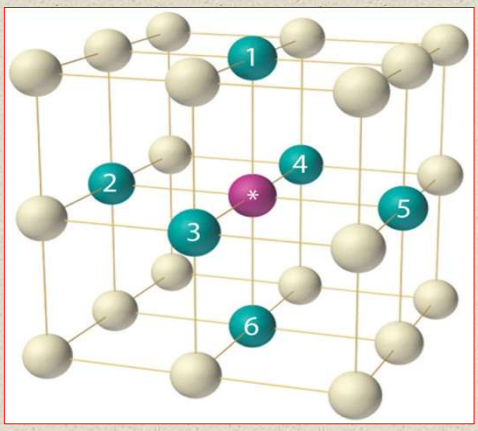
2.1 Metallic Structure



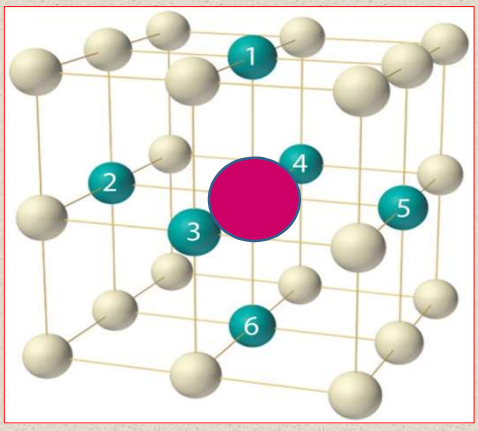
2.1 Metallic Structure

Coordination



2.1 Metallic Structure

Coordination



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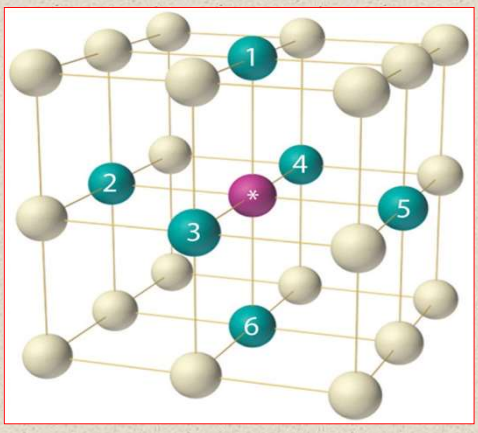
2.1 Metallic Structure

Coordination



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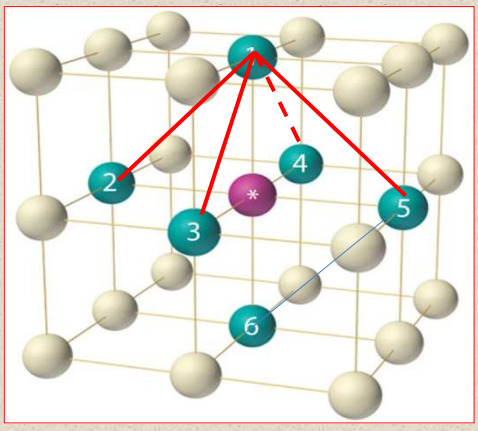
2.1 Metallic Structure

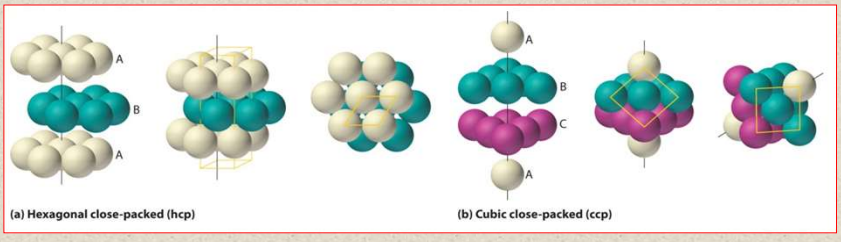
Coordination



2.1 Metallic Structure

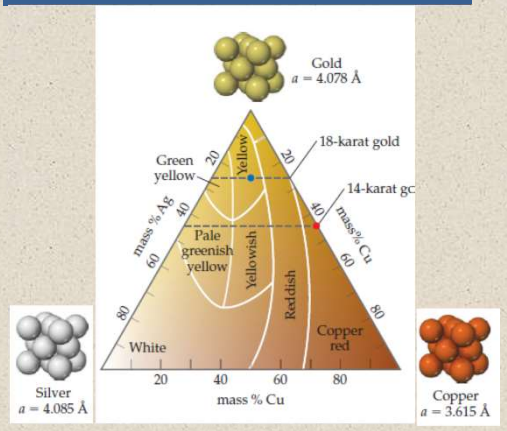
Coordination

Tructure	Percentage of Space Occupied by Atoms	Coordination Number
simple cubic	52	6
body-centered cubic	68	8
hexagonal close packed	74	12
cubic close packed	74	12



2.1 Metallic Structure

Alloy



2.1 Metallic Structure

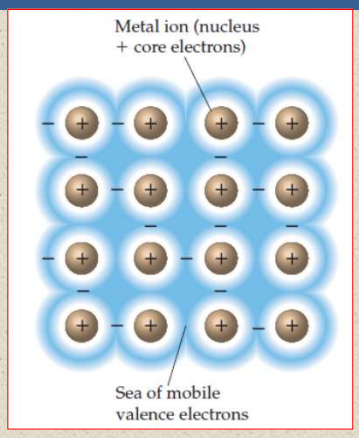
Alloy

Alloys categories:

1.substitutional alloys,
2.interstitial alloys,
3.heterogeneous alloys, and
4.intermetallic compounds

2.1 Metallic Structure

Bonding in metals: Electron-Sea Model



2.2 Ionic Compounds

The Caesium Chloride Structure (CsCl)

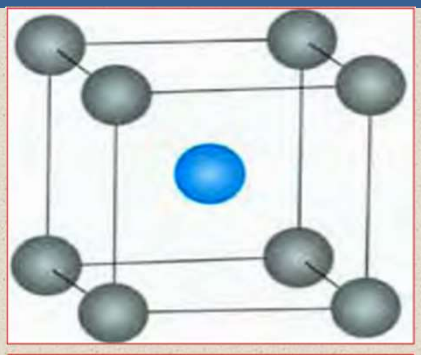
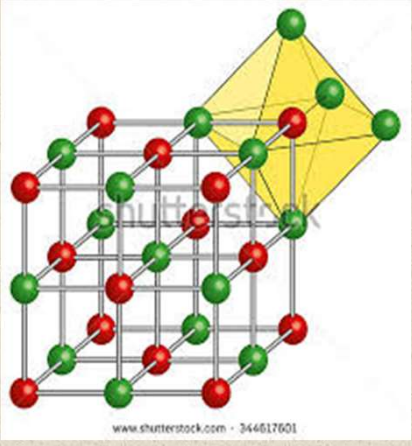


Figure 28. The CsCl unit cell. Cs, blue sphere; Cl, grey spheres (or vice versa).

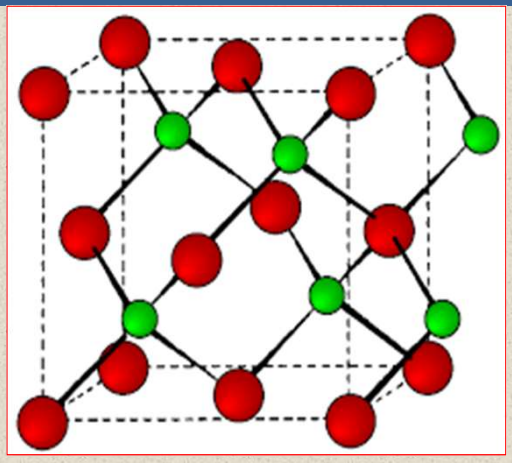
2.2 Ionic Compounds

The Sodium Chloride (or Rock Salt) Structure (NaCl)



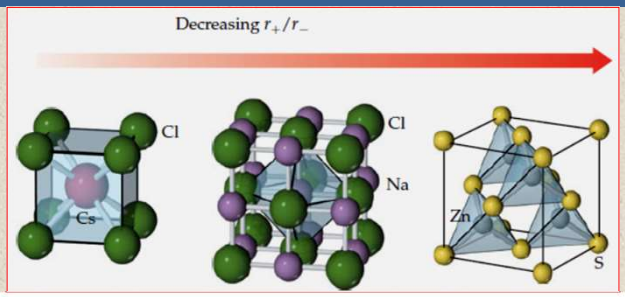
2.2 Ionic Compounds

The Zinc Blende Structures (ZnS)



2.2 Ionic Compounds

General remarks



	CsCl	NaCl	ZnS
Cation radius, r_+ (Å)	1.81	1.16	0.88
Anion radius, r_- (Å)	1.67	1.67	1.70
r_+/r_-	1.08	0.69	0.52
Cation coord. number	8	6	4
Anion coord. number	8	6	4

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