

## Chapter 1: Introduction

**Crystal:** Homogeneous solid possessing long-range three-dimensional internal order

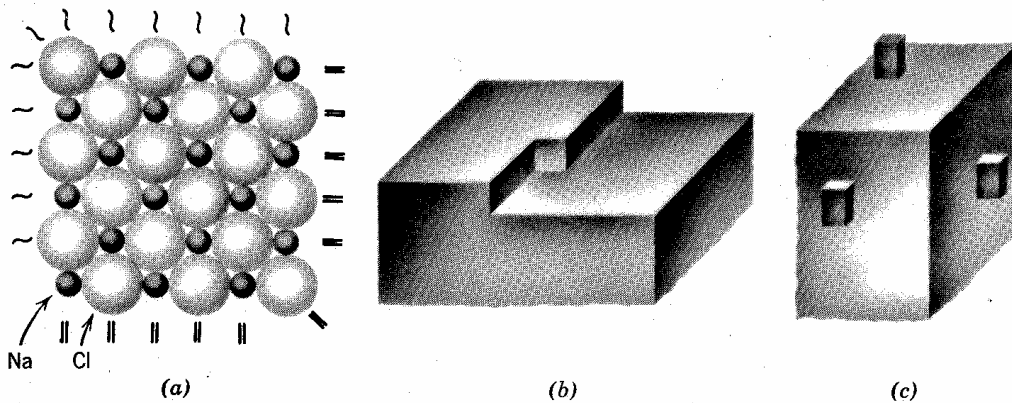
**Mineral:** A naturally occurring homogeneous solid with a definite (generally not fixed) chemical composition and a highly ordered-atomic arrangement usually formed by inorganic processes.

**Crystallisation:** A process when atoms in disordered state change to ordered arrangement characteristic of the crystalline state as the changing of temperature, pressure, and concentration.

Crystals can be formed from solutions, melts, and vapours.

**Crystal growth:** Nucleation and Critical size

FIG. 2.2. (a) A section through a corner of an NaCl crystal showing well-bonded, closely packed ions in the internal part of the crystal and unsatisfied chemical bonds at the outer surfaces of the crystal (~ represents unsatisfied and = represents satisfied chemical bonds). (b) A crystal surface showing a submicroscopic step. Attachment of ions at the location of such a step lowers the energy of the crystal surface. This energy is the cumulative result of the unsatisfied bonds. (c) Submicroscopic clumps of atoms, shown as blocks, attached to the outer three surfaces of a crystal. Such blocks create steps for the attachment of new layers of ions on the outer surfaces of the crystal.



### Internal structure of crystals

**Crystal structure.** Repetition of a motif or a group of atoms on a lattice or periodic array of points that orderly arrangement.

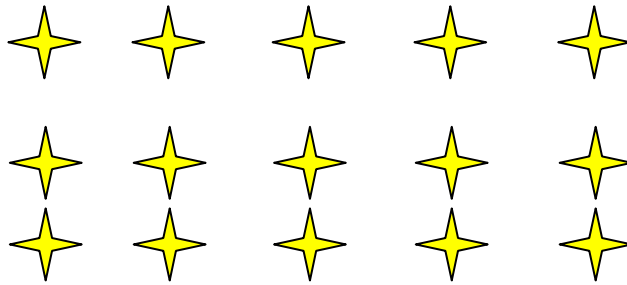
**Motif.** Group of atoms repeated on a lattice

**Lattice.** An imaginary patterns of points in which every point has an identical environment to that any other point in the pattern.

- Lattice point (One-dimensional order)

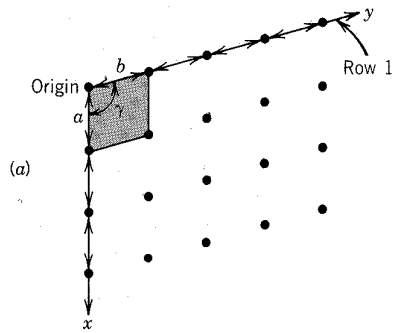


- Plane lattice (Two-dimensional order)



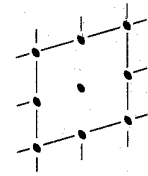
Five possible and distinct plane lattices

1. Oblique lattice
2. Rectangular lattice
3. Centre rectangular & Diamond lattice
4. Hexagonal lattice
5. Square lattice

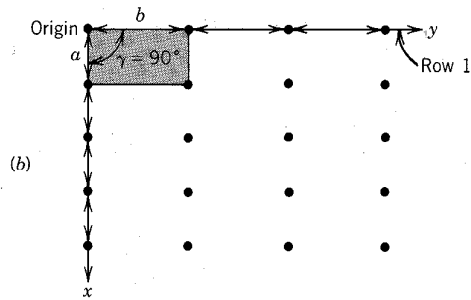


**Oblique net**

$a \neq b$   
 $\gamma \neq 90^\circ$

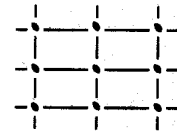


**p2**

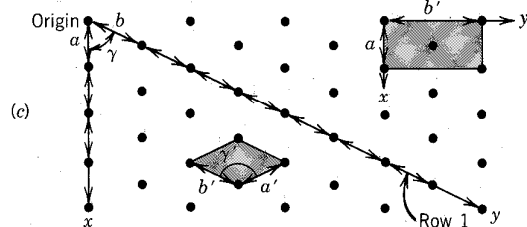


**Rectangular net**

$a \neq b$   
 $\gamma = 90^\circ$

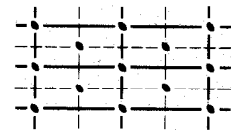


**p2mm**



**Centered rectangular net**

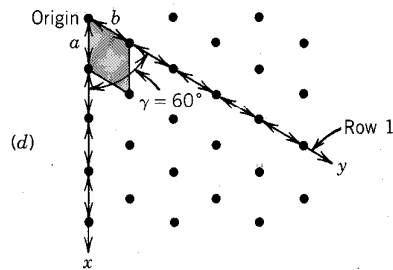
$\cos \gamma = \frac{a}{2b}$   
 $a \neq b$



**c2mm**

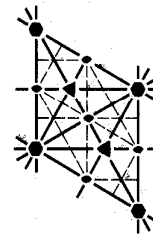
**Diamond net**

$a' = b'$   
 $\gamma' \neq 90^\circ, 60^\circ,$   
 or  $120^\circ$

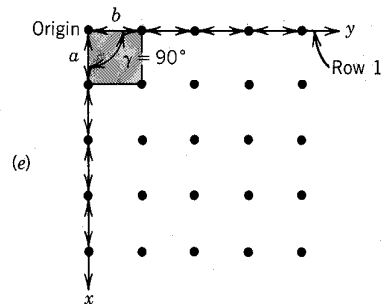


**Hexagonal net**

$a = b$  (or  $a_1 = a_2$ )  
 $\gamma = 60^\circ$

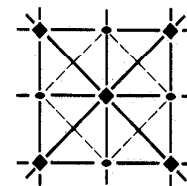


**p6mm**



**Square net**

$a = b$  (or  $a_1 = a_2$ )  
 $\gamma = 90^\circ$



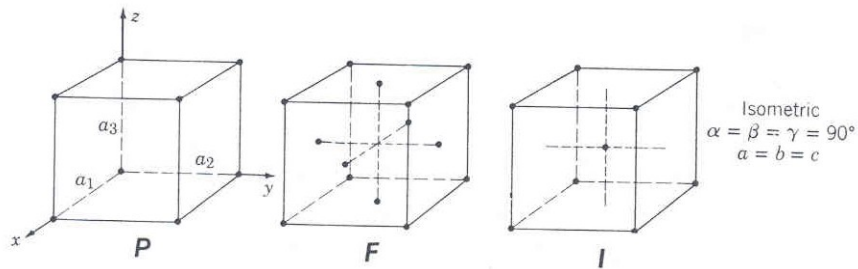
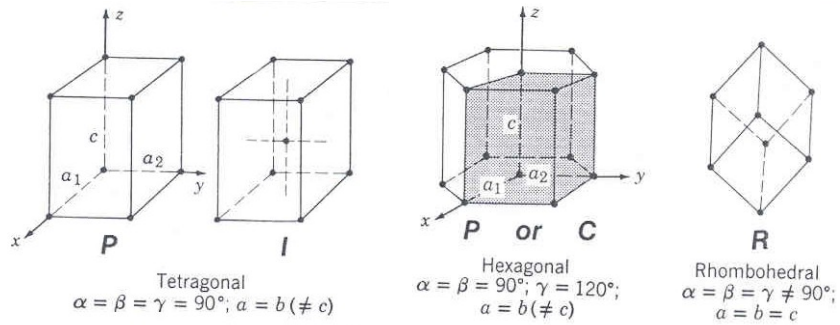
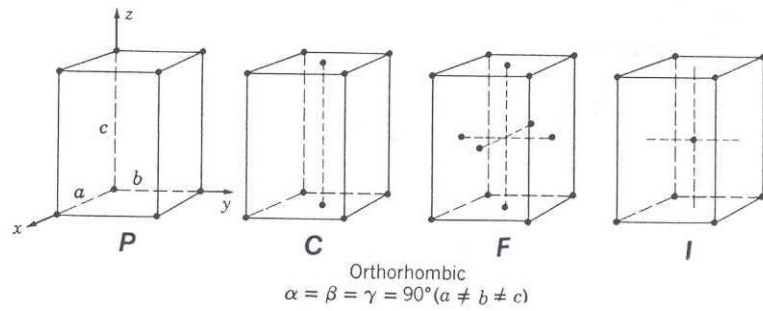
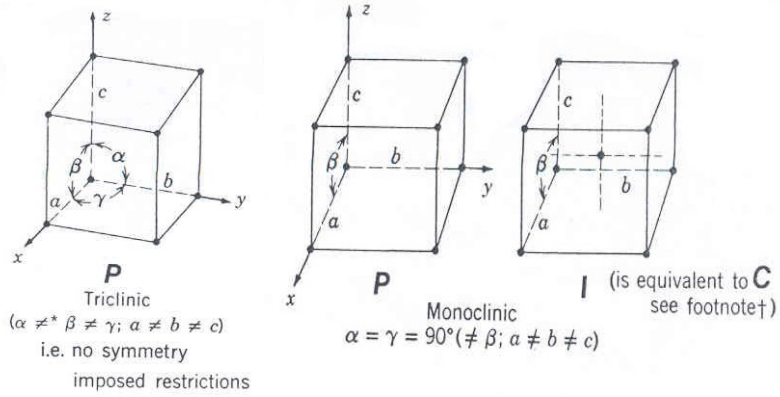
**p4mm**

FIG. 3.5 Development of the five distinct plane lattices (or nets) by the indefinite repeat of a row (along direction  $y$ , with specified translation distance  $b$ ), along direction  $x$  with repeat distance  $a$ ;  $\gamma$  is the angle between  $x$  and  $y$ . The total symmetry content of each of the unit cell choices is given in the right-hand column. Rotational axes are shown by standard symbols, mirrors by broad lines, and glide lines by dashed lines.

\*The sign  $\neq$  implies non-equality by reason of symmetry; accidental equality may occur.

- Space lattice (Three-dimensional order)

14 Bravais lattices



*Unit cell:* The smallest units of repeat in these lattices outline the unit cells.

- Primitive unit cell
- Non-primitive unit cell

*Type of 3D unit cells:* Primitive unit cell (P)

Base-centred unit cell (C)

Body-centred unit cell (I)

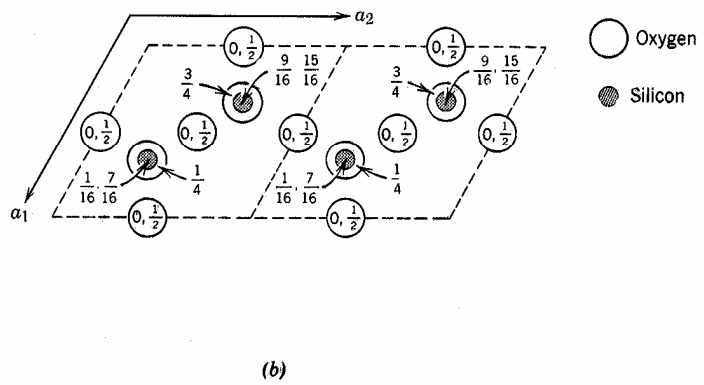
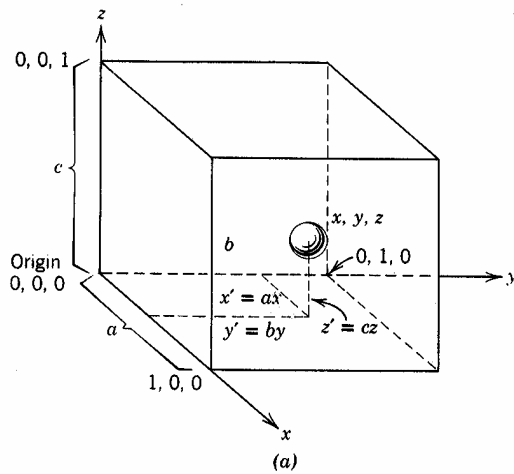
Face-centred unit cell (F)

*Structural types based on close-packing*

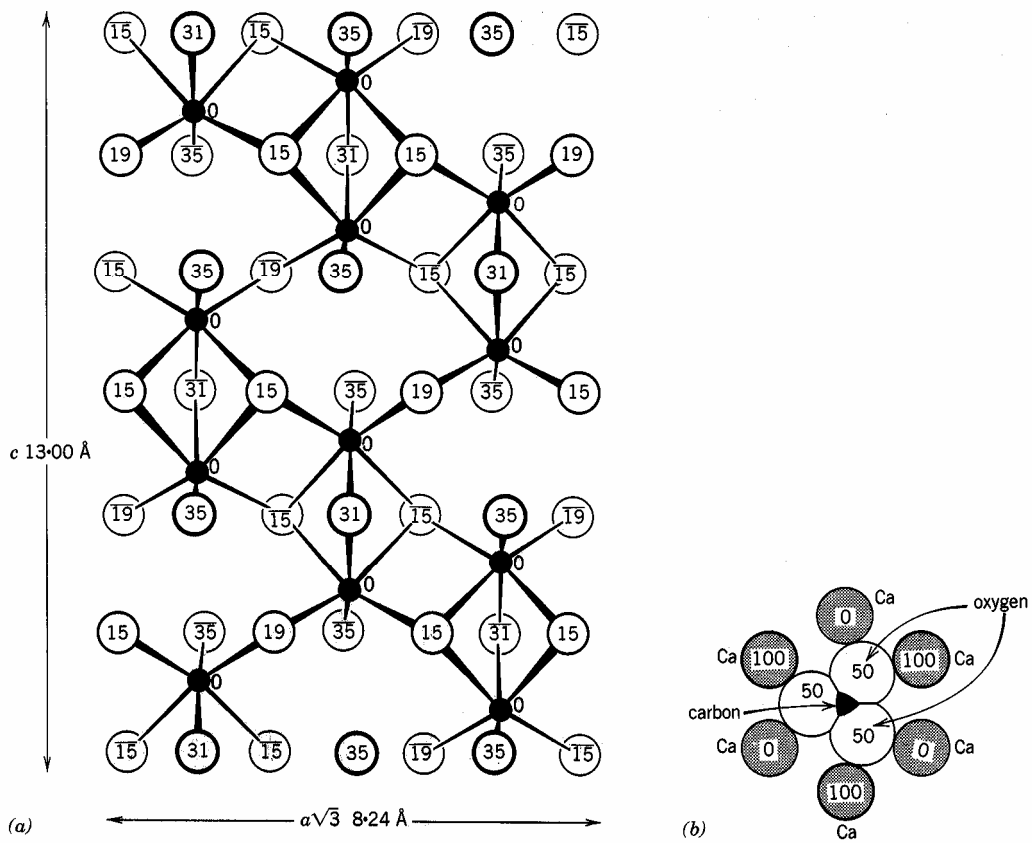
- hexagonal close-packing
- cubic close-packing
- body-centred cubic close packing

*Illustration of crystal structure*

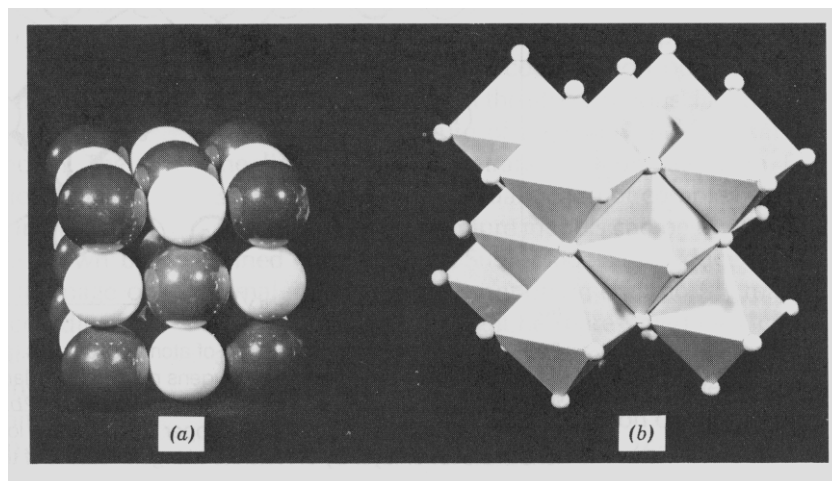
- Fractional cell coordination (x, y, z)



- Atomic position with numbers (0-100)



- A close-packing model & Polyhedral model

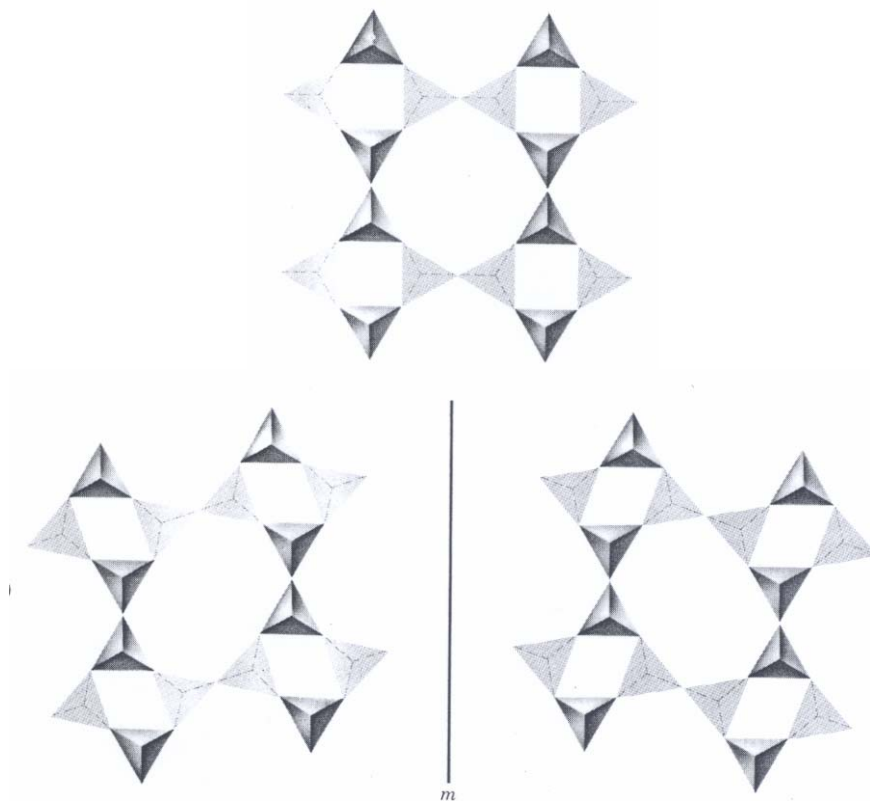


*Isomorphism*: Crystals in which the centres of constituent atoms occupy geometrically similar position, regardless the size of atoms or absolute dimension of the structure.

Mineral	Chemical Composition	Cation Size* (Å)	Unit Cell Dimensions (Å)			Volume (Å <sup>3</sup> )	Specific Gravity (G)	Cleavage Angle $110 \wedge 1\bar{1}0$
			<i>a</i>	<i>b</i>	<i>c</i>			
Aragonite	CaCO <sub>3</sub>	Ca <sup>2+</sup> 1.18	4.96	7.97	5.74	226.91	2.94	63°48'
Strontianite	SrCO <sub>3</sub>	Sr <sup>2+</sup> 1.45	5.11	8.41	6.03	259.14	3.78	62°41'
Cerussite	PbCO <sub>3</sub>	Pb <sup>2+</sup> 1.49	5.19	8.44	6.15	269.39	6.58	62°46'
Witherite	BaCO <sub>3</sub>	Ba <sup>2+</sup> 1.47	5.31	8.90	6.43	303.87	4.31	62°12'

\*Because the metal ions are coordinated to 9 oxygens, the ionic radii (see page 188) are given for 9-fold coordination.

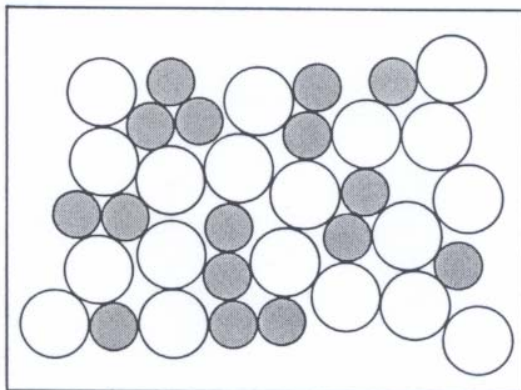
*Polymorphism*: The ability of a specific chemical substance to crystallise with more than one type of structure (as a function to the changing of temperature and pressure).



Composition	Mineral Name	Crystal System and Space Group	Hardness	Specific Gravity
C	Diamond	Isometric— $Fd\bar{3}m$	10	3.52
	Graphite	Hexagonal— $P6_3/mmc$	1	2.23
FeS <sub>2</sub>	Pyrite	Isometric— $Pa\bar{3}$	6	5.02
	Marcasite	Orthorhombic— $Pnmm$	6	4.89
CaCO <sub>3</sub>	Calcite	Rhombohedral— $R\bar{3}c$	3	2.71
	Aragonite	Orthorhombic— $Pnam$	3½	2.94
SiO <sub>2</sub>	Low quartz	Hexagonal— $P3_121$	7	2.65
	High quartz	Hexagonal— $P6_222$		2.53
	High tridymite	Hexagonal— $P6_3/mmc$	7	2.20
	High cristobalite	Isometric— $Fd\bar{3}m$	6½	2.20
	Coesite	Monoclinic— $C2/c$	7½	3.01
	Stishovite	Tetragonal— $P4_2/mnm$		4.30

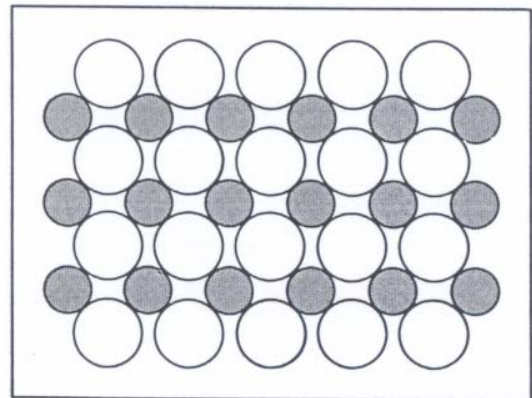
*Mineraloid* (Noncrystalline minerals): Natural occurring amorphous substance

Amorphous: Substance that lack of internal atoms arrangement.



(a)

Amorphous alloy



(b)

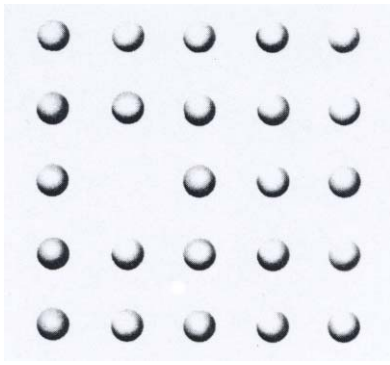
Crystalline alloy

*Pseudomorphism*: The existence of a mineral with the outward crystal form of another mineral species.

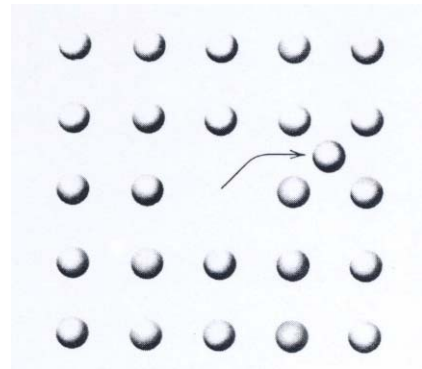
1. Substitution
2. Encrustation
3. Alteration

*Structural complexities and defects*

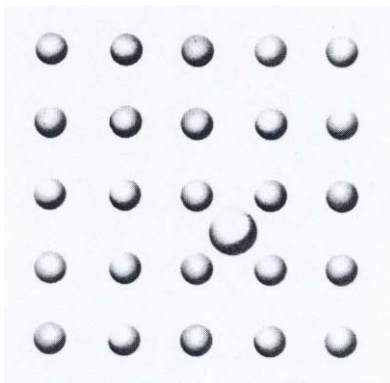




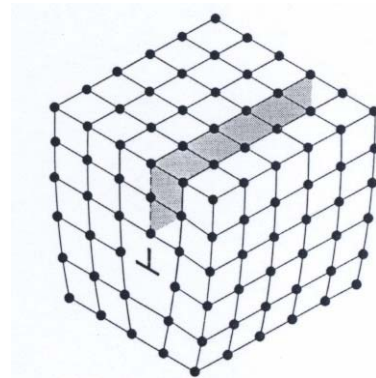
Schottky defect



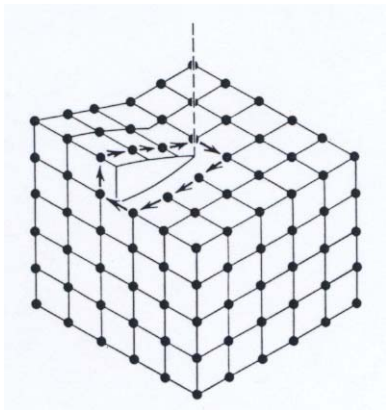
Frenkel defect



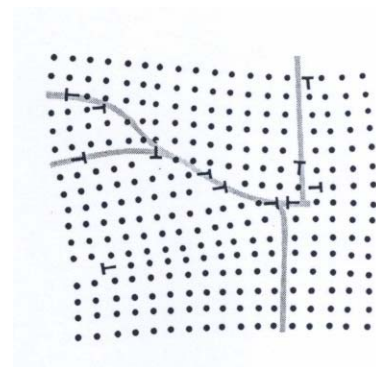
Impurity defect (interstitial)



Edge dislocation



Screw dislocation



Lineage structure