MATERIAL SCIENCE & ENGINEERING (20A03201T)

Mr. P KUMAR., M-Tech (PhD)
Assistant Professor
Department of Mechanical Engineering
VEMU Institute of Technology

Course Objectives

- To teach the principles of physical metallurgy, i.e. crystallography of metals, constitution of alloys, phase diagrams.
- Expose commercially important metals and alloys (both ferrous and non ferrous) with engineering constraints.
- Explain the methods to change the properties of materials through heat treatment processes
- Familiarize properties and applications of ceramics, polymers and composite materials.
- Demonstrate the fundamental properties of nano-materials and their applications.

Course Outcomes:

- After completing the course, the student will be able to

- Explain the principles of binary phases. (l2)
- Select steels and cast irons for a given application. (l3)
- Apply heat treatment to different applications. (l3)
- Utilize nonferrous metals and alloys in engineering. (l3)
- Choose composites for various applications. (l3)
- Assess the properties of nano-scale materials and their applications. (l2)
- Differentiate between hardening of ferrous and non-ferrous alloys. (L4)

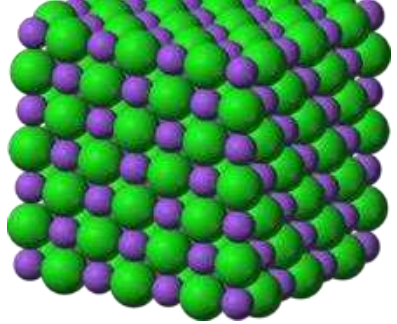
UNIT -I

- Structure of Metals: Crystal Structures: Unit cells, Metallic crystal structures, Imperfection in solids: Point, Line, interstitial and volume defects; dislocation strengthening mechanisms and slip systems, critically resolved shear stress.
- Constitution of Alloys: Necessity of Alloying, substitutional and interstitial solid solutions- Phase diagrams: Interpretation of binary phase diagrams and microstructure development; eutectic, peritectic, peritectoid and monotectic reactions. Iron-Iron-carbide diagram and microstructural aspects of ferrite, cementite, austenite, ledeburite, and cast iron.

Learning Outcomes:

- At the end of this unit the student will be able to
- Understand the importance of material science in engineering.(l2)
- Recall the definitions and terminology of crystallography. (l1)
- Distinguish metals and alloys. (l4)
- Make use of the principles of construction of binary phase diagrams. (l3)
- Identify various invariant reactions in binary phase diagrams. (l3)
- Know the concept of metallography in studying the microstructures of metals and alloys. (l2)

Crystal structure



- ✓ In crystallography, crystal structure is a description of the ordered arrangement of atoms, ions or molecules in a crystalline material.
- ✓ Ordered structures occur from the intrinsic nature of the constituent particles to form symmetric patterns that repeat along the principal directions of three-dimensional space in matter.

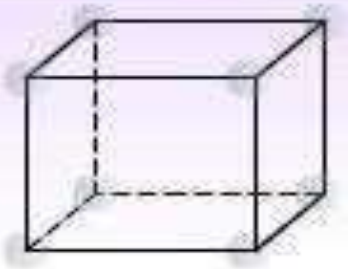
- ✓The smallest group of particles in the material that constitutes this repeating pattern is the unit cell of the structure.
- ✓The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principal axes.
- ✓The translation vectors define the nodes of the Bravais lattice.

- ✓The lengths of the principal axes, or edges, of the unit cell and the angles between them are the lattice constants, also called lattice parameters or cell parameters.
- ✓The symmetry properties of the crystal are described by the concept of space groups. All possible symmetric arrangements of particles in three-dimensional space may be described by the 230 space groups.
- ✓The crystal structure and symmetry play a critical role in determining many physical properties, such as cleavage, electronic band structure, and optical transparency.

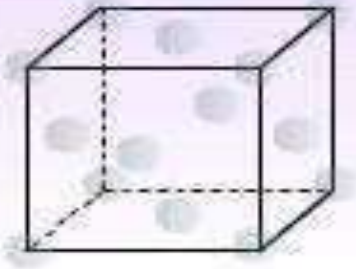
Unit Cells Types

A unit cell is the smallest component of the crystal that reproduces the whole crystal when stacked together with purely translational repetition.

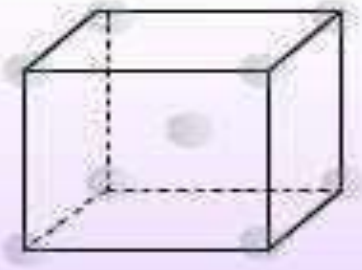
- Primitive (P) unit cells contain only a *single lattice point.*
- Internal (I) unit cell contains an atom in the *body center.*
- Face (F) unit cell contains atoms in the *all faces of the planes* composing the cell.
- Centered (C) unit cell contains atoms *centered on the sides* of the unit cell.



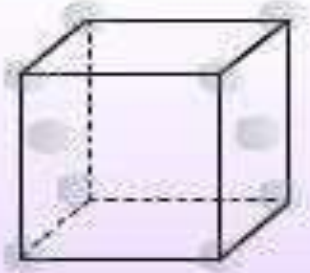
Primitive



Face-Centered



Body-Centered



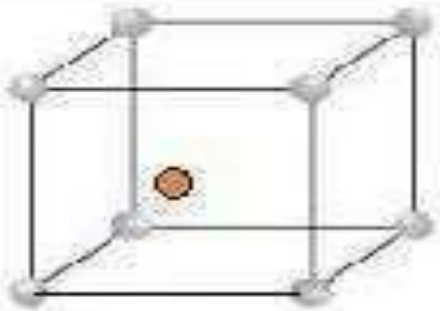
End-Centered

Centred Unit Cell

(Particles are present at the corners as well as other position)

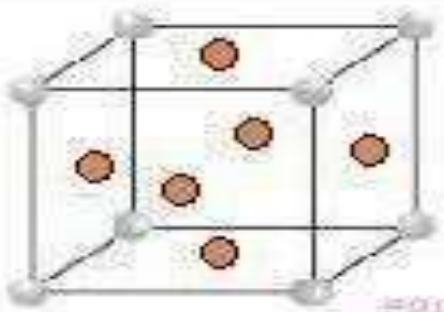
Body - Centred

Contains one particle at centre of body



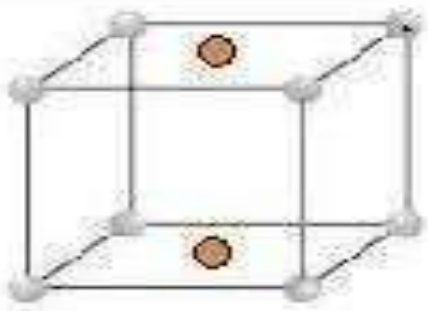
Face - Centred

Contains one particle at centre of each of the face

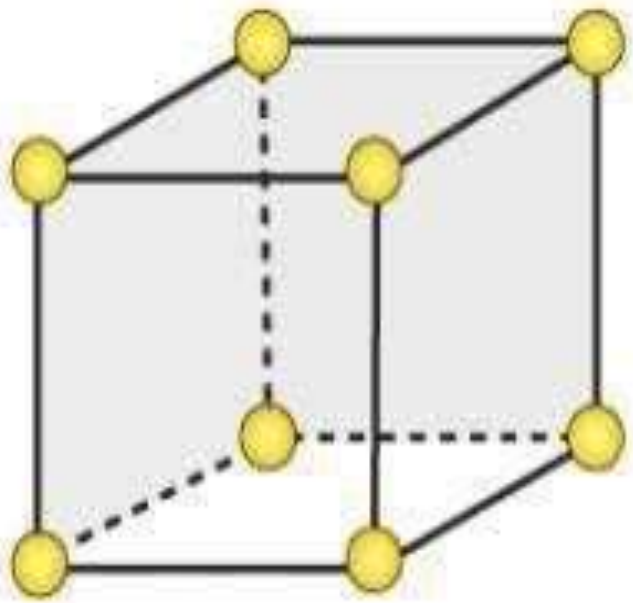


End - Centred

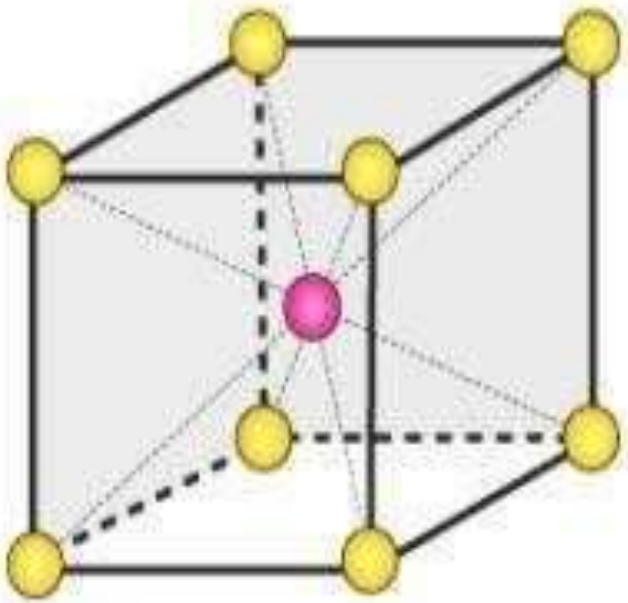
Contains one particle at center of any two oppoing face



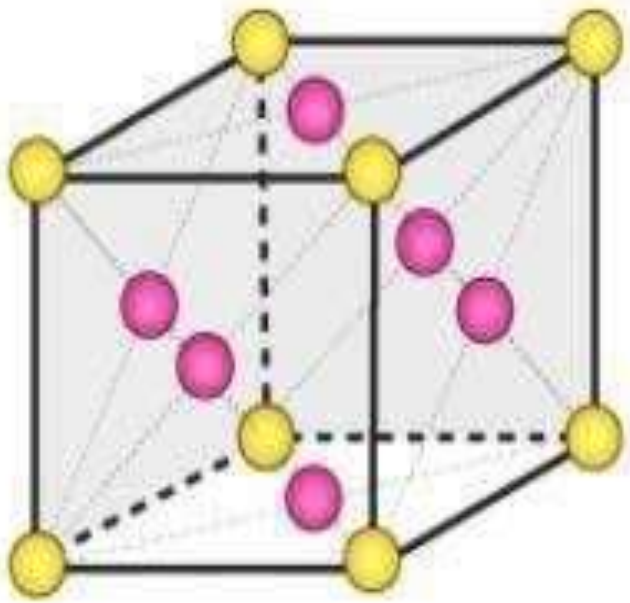
TYPES OF UNIT CELL



Simple cubic

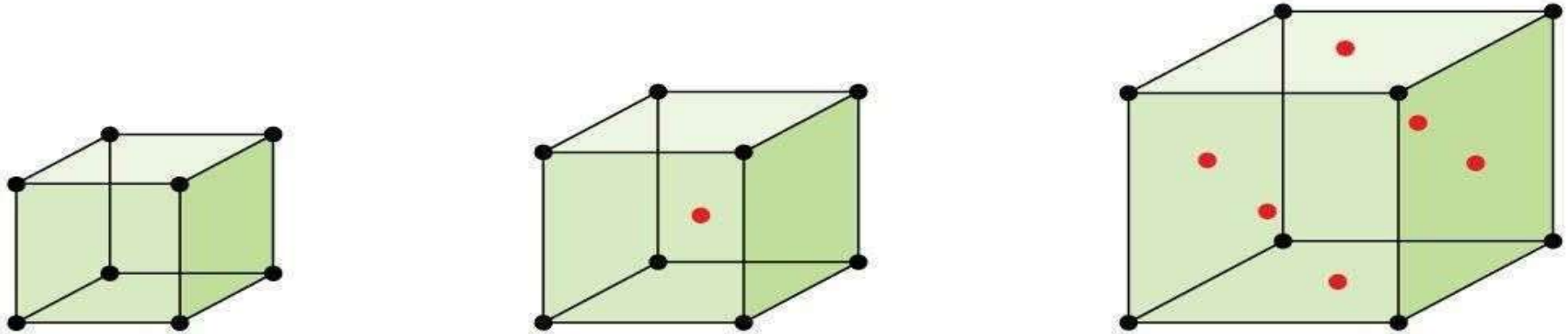


Body-centred Cubic Unit Cell (BCC)

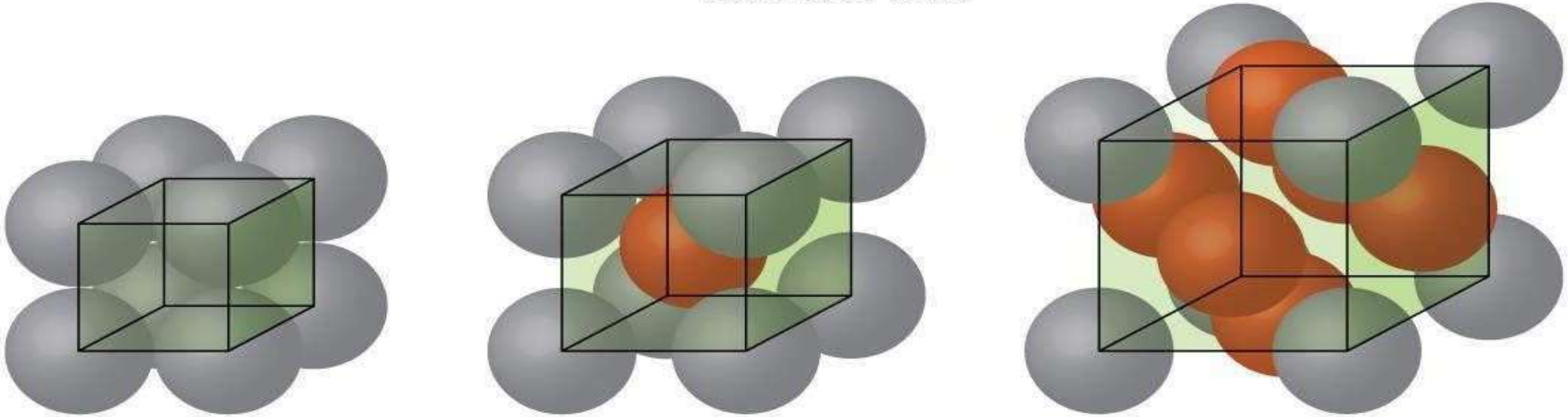


Face-centred Cubic Unit Cell (FCC)

Lattice point locations



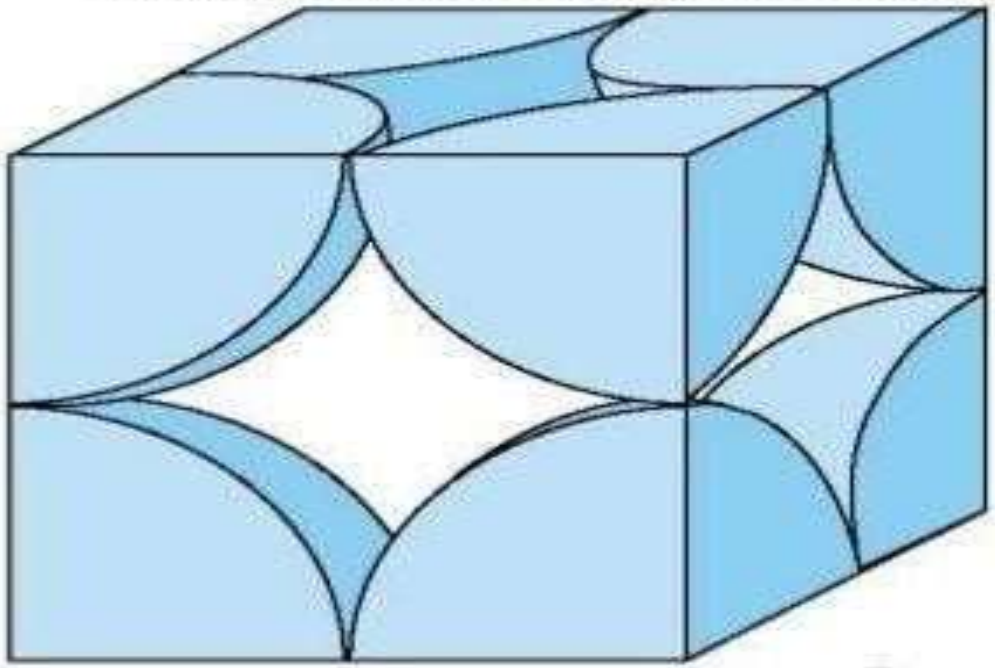
Cubic unit cells



Simple cubic | Body-centered cubic | Face-centered cubic

SIMPLE CUBIC (SC)

- The atoms lie on a grid: layers of rows and columns.
- Sit at the corners of stacked cubic

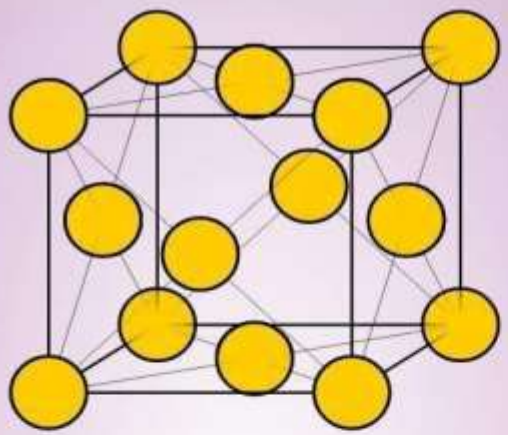


No. of atom at corner
= 8 x 1/8 = 1 atom

Total No. of atom in one unit cell
= 1 atom

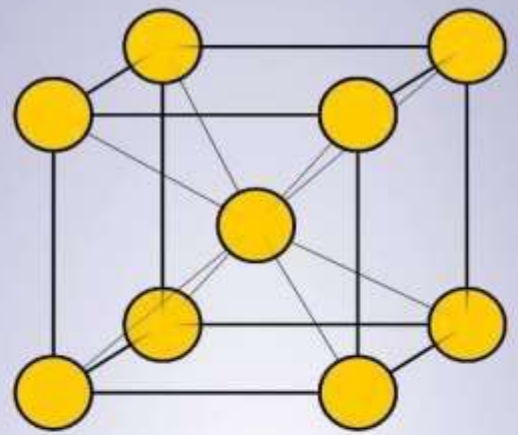
Example : Manganese

Crystal Structure	FCC	BCC
Unit Cell Type	Cubic	Cubic
Relationship Between Cube Edge Length *a* and the Atomic Radius *R*	$a = 2R\sqrt{2}$	$a = 4R/\sqrt{3}$
Close-Packed Structure	Yes	No
Atomic Packing Factor (APF)	74%	68%
Coordination Number	12	8
Number of Atoms per Unit Cell	4	2
Number of Octahedral Interstitial Sites	4	6
Number of Tetrahedral Interstitial Sites	8	12



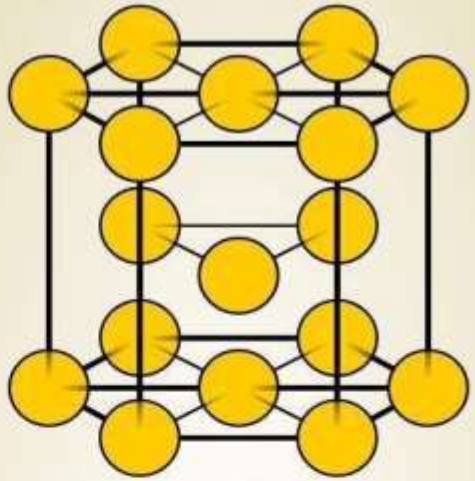
Examples of **FCC** elements at room temperature:

Al, Ca, **Ni**, **Cu**, Sr, Rh, **Pd**, **Ag**, Yb, Th, **Ir**, **Pt**, **Au**, **Pb**



Examples of **BCC** elements at room temperature:

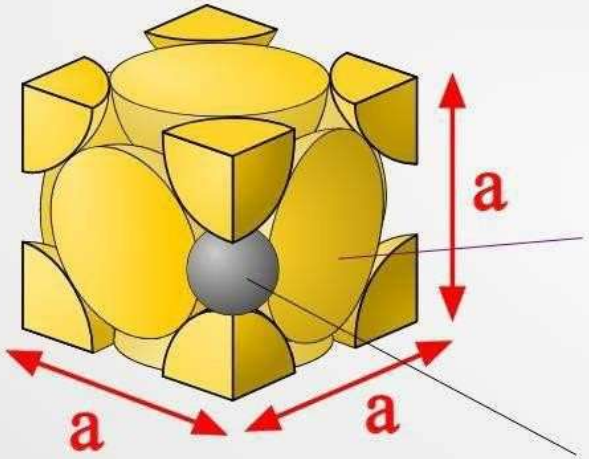
Li, **Na**, **K**, **V**, **Cr**, **Mn**, **Fe**, Rb, **Nb**, **Mo**, Cs, Ba, Eu, **Ta**, **W**, Ra



Examples of **HCP** elements at room temperature:

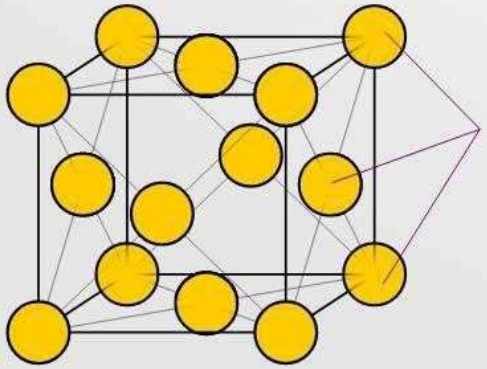
Be, **Mg**, Sc, **Ti**, **Co**, **Zn**, Y, **Zr**, Tc, Ru, Cd, Gd, Tb, Dy, Ho, Er, Tm, Lu, Hf, Re, Os, Tl

Austenite



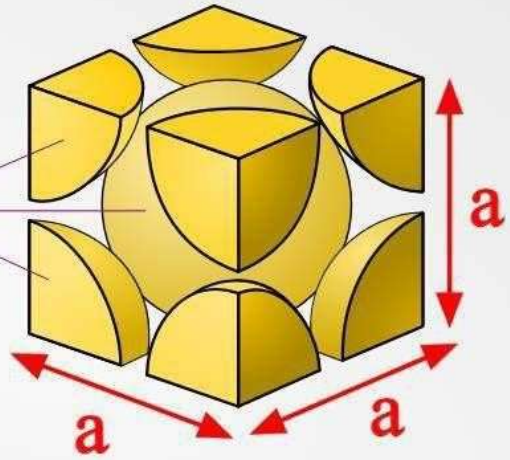
Fe

C

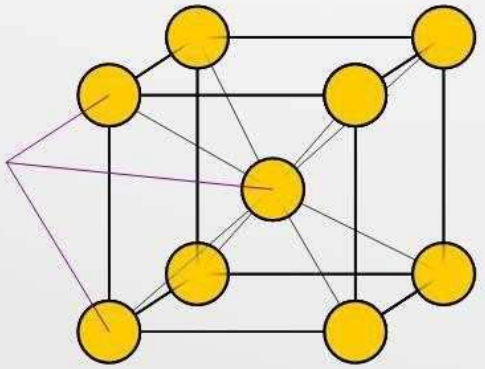


Face-Centered
Cubic **FCC**

Ferrite



Iron (Fe)
atoms



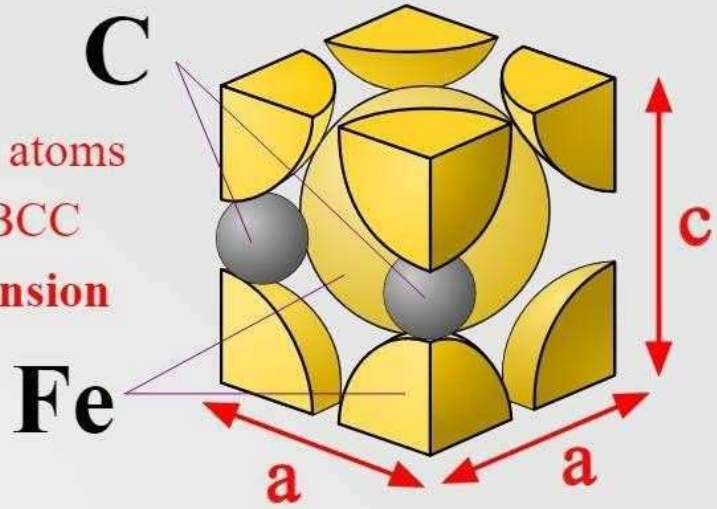
Body-Centered
Cubic **BCC**

Martensite

C

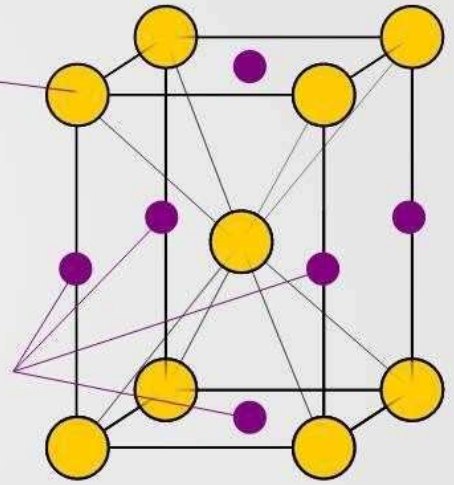
Extra carbon atoms
cause the BCC
lattice expansion

Fe

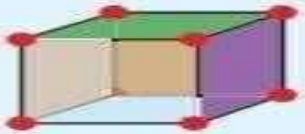
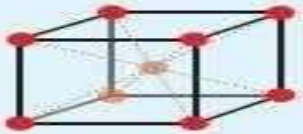
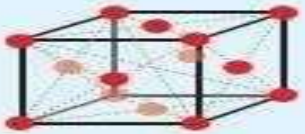
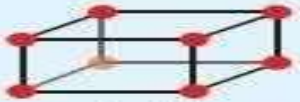
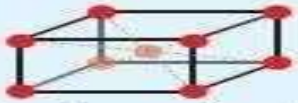
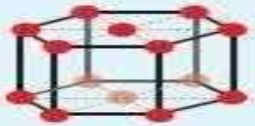
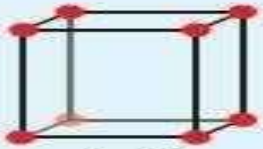
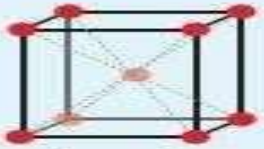
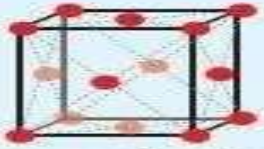
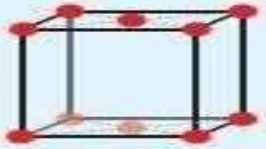
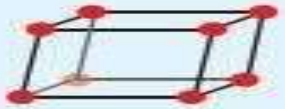
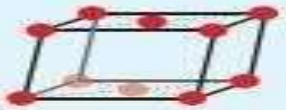
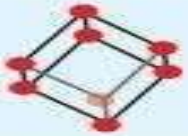
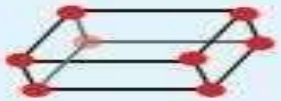


Iron (Fe)
atoms

Sites that might
be occupied by
carbon atoms



Body-Centered
Tetragonal **BCT**

cubic	 primitive	 body centered	 face centered
tetragonal	 primitive	 body centered	
hexagonal			
orthorhombic	 primitive	 body centered	 face centered  basis face centered
monoclinic	 primitive		 basis face centered
trigonal			
triclinic			

Crystal Structures of Metals

- All metallic elements (except Cs, Ga, and Hg) are crystalline solids at room temperature. Like ionic solids, metals and alloys have a very strong tendency to crystallize, whether they are made by thermal processing or by other techniques such as solution reduction or electroplating.
- Metals crystallize readily and it is difficult to form a glassy metal even with very rapid cooling.
- gallium, and mercury are the only three **metals** that are liquid at or around room temperature

Crystal Structures of Metals

- Molten metals have low viscosity, and the identical (essentially spherical) atoms can pack into a crystal very easily.
- Glassy metals can be made, however, by rapidly cooling alloys, particularly if the constituent atoms have different sizes.
- The different atoms cannot pack in a simple unit cell, sometimes making crystallization slow enough to form a glass.
- Most metals and alloys crystallize in one of three very common structures: body-centered cubic (bcc), hexagonal close packed (hcp), or cubic close packed (ccp, also called face centered cubic, fcc). In all three structures the coordination number of the metal atoms (i.e., the number of equidistant nearest neighbors) is rather high: 8 for bcc, and 12 for hcp and ccp.

Crystal Structures of Metals

- We can contrast this with the low coordination numbers (i.e., low valences - like 2 for O, 3 for N, or 4 for C) found in nonmetals.
- In the bcc structure, the nearest neighbors are at the corners of a cube surrounding the metal atom in the center. In the hcp and ccp structures, the atoms pack like stacked cannonballs or billiard balls, in layers with a six-coordinate arrangement.
- Each atom also has six more nearest neighbors from layers above and below. The stacking sequence is ABCABC... in the ccp lattice and ABAB... in hcp. In both cases, it can be shown that the spheres fill 74% of the volume of the lattice.

WHY STUDY IMPERFECTIONS IN SOLIDS?

(page 144)

Important to have knowledge on types of imperfections and roles they play in affecting the behavior of metals.

Properties of materials are influenced by the presence of imperfections.

Mechanical properties of pure metals change significantly when metals are alloyed.

Yield Strength of Pure Copper (Cu): 117 MPa

Yield Strength of Brass (70% Cu & 30% Zn): 200 MPa

Imperfection in solids

For a crystalline solid we have assumed that perfect order exists throughout the material on an atomic scale.

However, such an idealized solid does not exist.

All contain large numbers of various defects or imperfections. The influence of the imperfections is not always adverse.

Specific characteristics are fashioned by the introduction of the controlled amount or number of particular defect.

Classification of crystalline imperfection : according to the geometry and dimensionality of the defect.

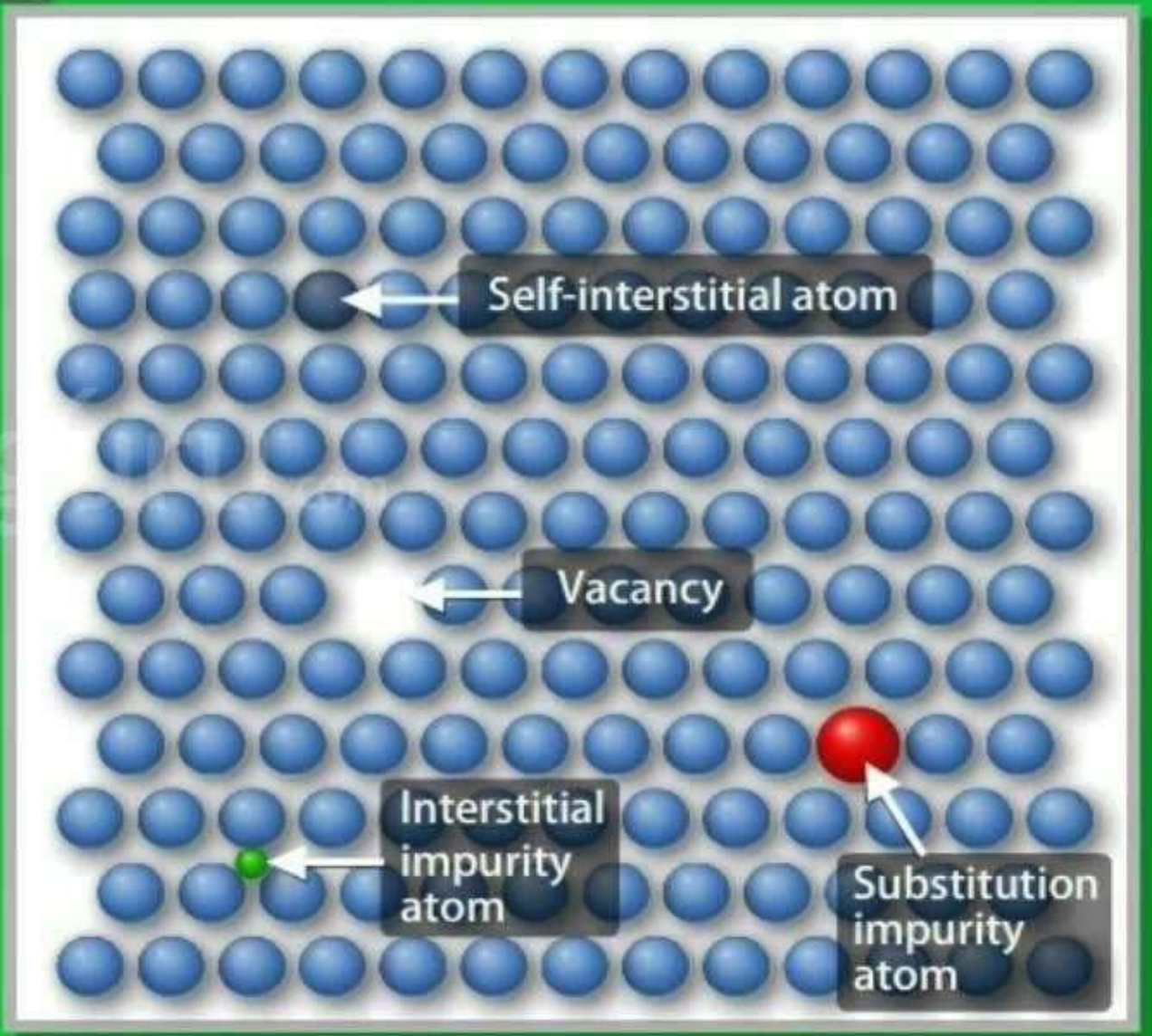
Point defect: associated with one or two atomic positions
Linear defect: one dimensional defect
Interfacial defect or boundaries: two dimensional defect
Impurities in solid: as point defect

CLASSIFICATION OF DEFECTS BASED ON DIMENSIONALITY

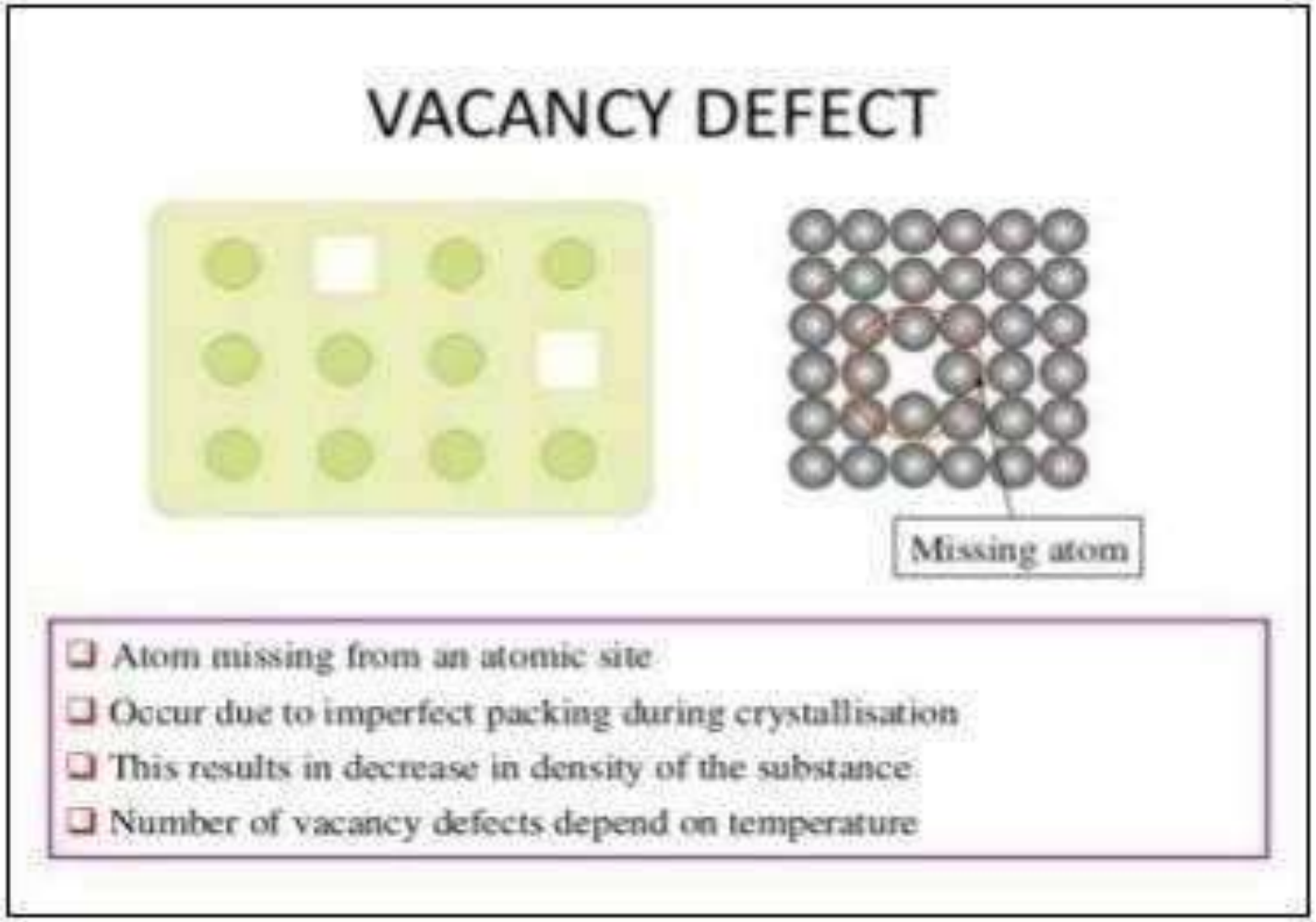
- **0D (*Point defects*)**
  - Vacancy
  - Interstitial
  - Frenkel defect
  - Schottky defect
- **1D (*Line defects*)**
  - Edge Dislocation
  - Screw Dislocation
- **2D (*Surface / Interface*)**
  - Grain boundary
  - Twin boundary
  - Stacking faults
- **3D (*Volume defects*)**
  - Dispersant
  - Precipitate
  - Inclusion
  - Voids / Cracks

Types of Point Defects

Point defects are the irregularities or deviations from ideal arrangement around a point or an atom in a crystalline substance, whereas the line defects are the irregularities or deviations from ideal arrangement in entire rows of lattice points. These irregularities are called crystal defects.



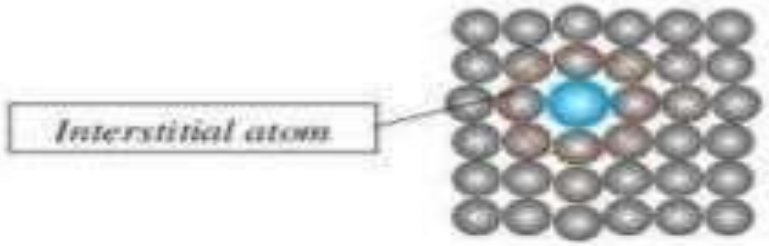
Vacancy defect: It is the simplest point defect. In this system, an atom is missing from its regular atomic site. Vacancies are formed during solidification due to vibration of atoms.



INTERSTITIAL DEFECT

Atoms which occupy a site in the crystal structure at which there is usually not an atom, or two or more atoms sharing one or more lattice sites such that the number of atoms is larger than the number of lattice sites.

INTERSTITIALS DEFECT

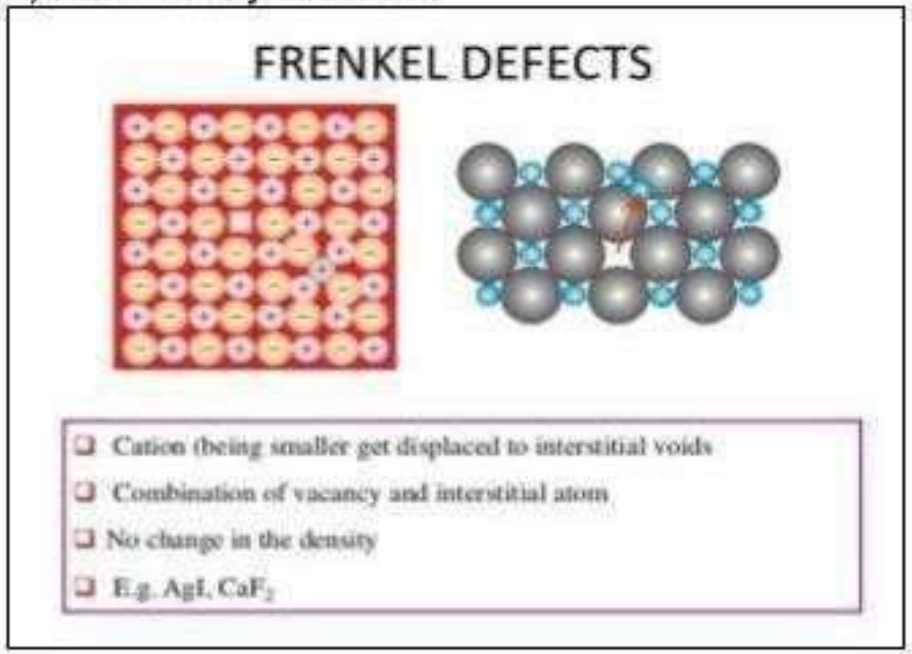


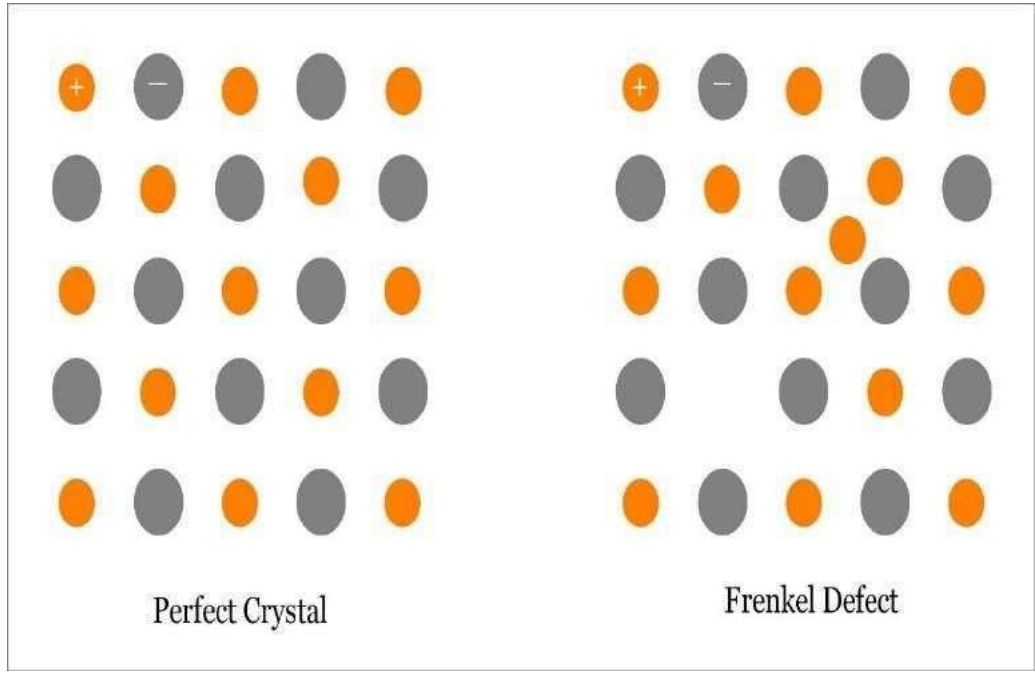
- Addition of an extra atom within a crystal structure
- This defect increases the density of the substance
- Causes atomic distortion
- Vacancy and interstitials are inverse phenomena

FRENKEL DEFECT

A Frenkel defect is also known as Frenkel pair or Frenkel disorder, it is a type of point defect in a crystal lattice.

The defect forms when an atom or smaller ion(usually cation) leaves its place in the lattice, creating a vacancy, and becomes an interstitial by lodging (accommodation) in a nearby location.





SCHOTTKY DEFECT

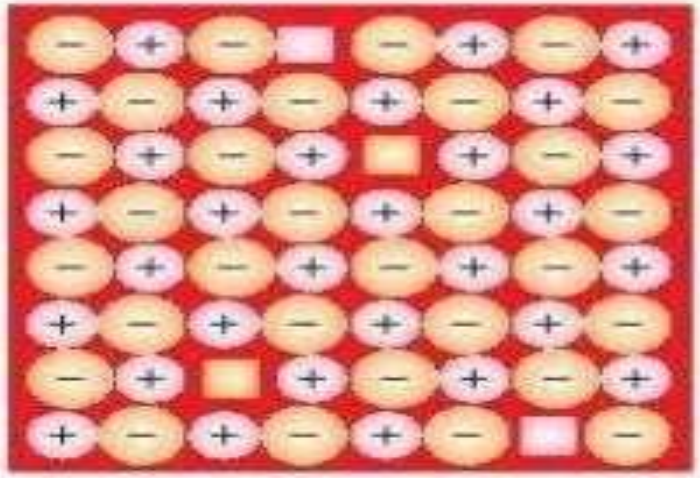
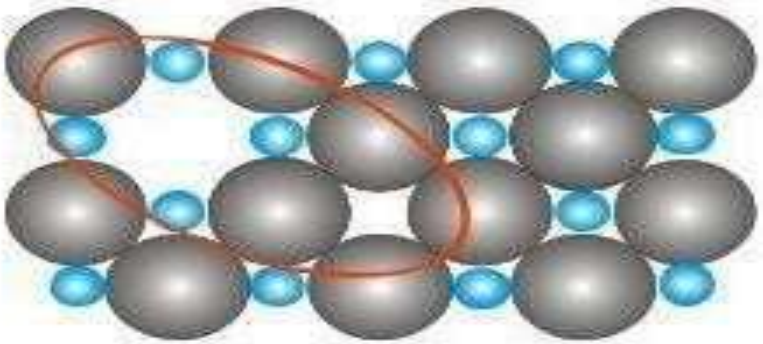


Fig. 1.26: Schottky defects



- Pair of anion and cation vacancies
- In order to maintain electrical neutrality, the number of missing cations and anions are equal
- It also decreases the density of crystal
- E.g. Alkali halides such as NaCl, KF, etc.

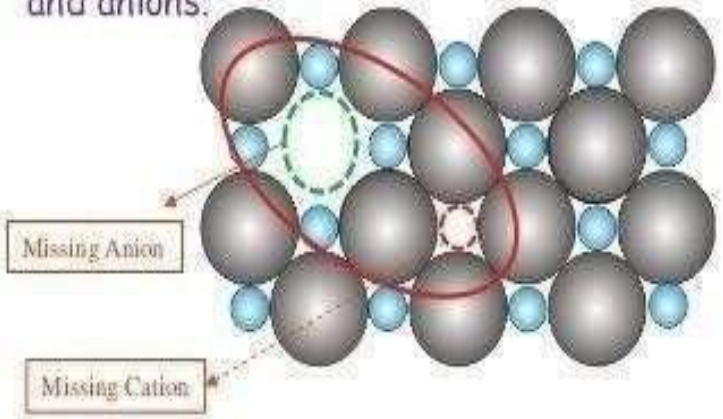
Schottky defect and Frenkel defect

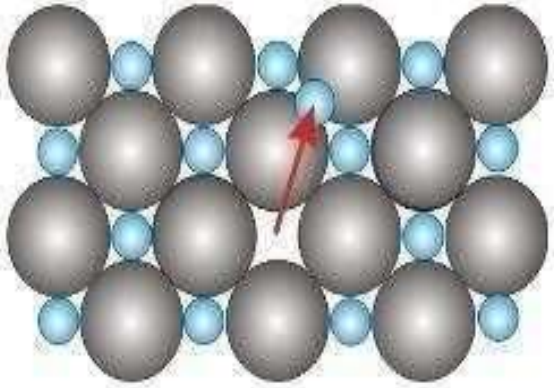
Schottky Defect:

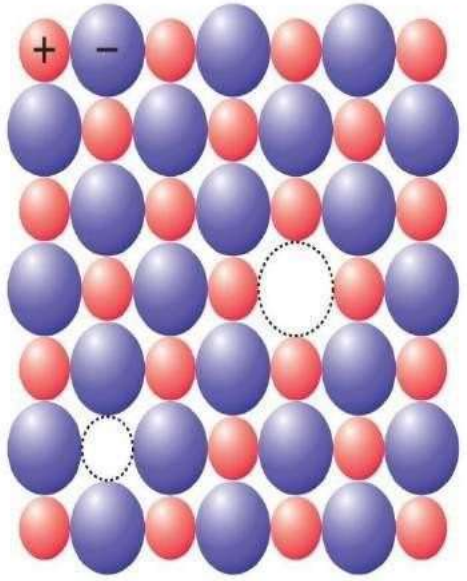
- Forms when oppositely charged ions leave their lattice sites, creating vacancies.
- These vacancies are formed in stoichiometric units, to maintain an overall neutral charge in the ionic solid.
- Density of the solid crystal is less than normal
- Occurs only when there is small difference in size between cations and anions.

Frenkel Defect:

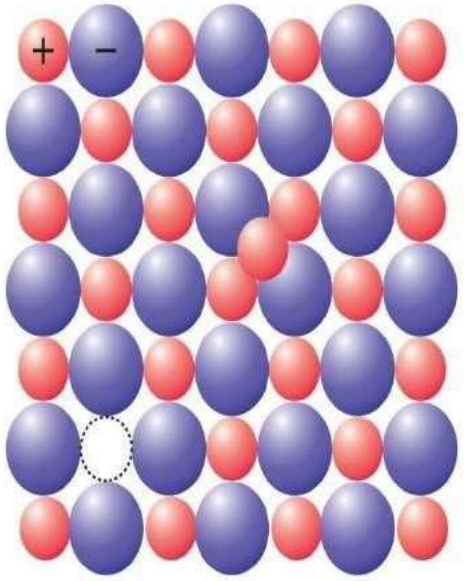
- Smaller ion (usually the cation) is displaced from its lattice position to an interstitial site.
- Creates a **vacancy defect** at its original site and an **interstitial defect** at its new location.
- Does not change the density of the solid.
- Shown in ionic solids with large size difference between the anion and cation.







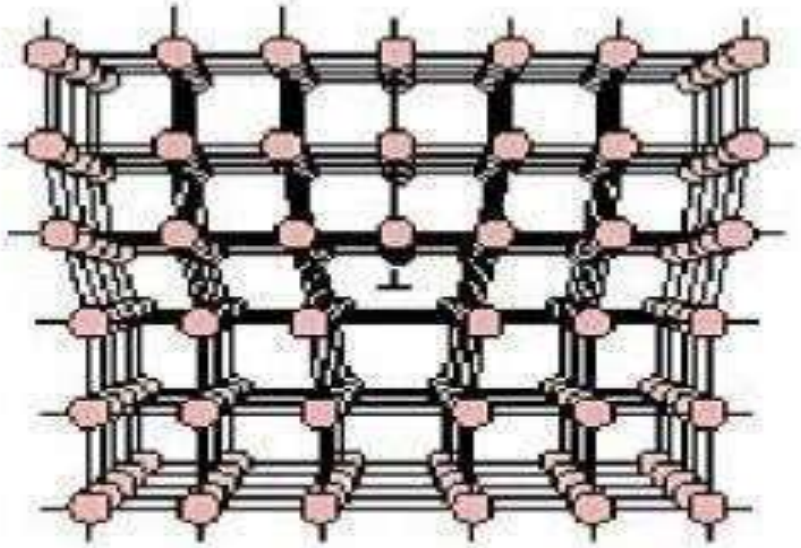
(a) Schottky defect



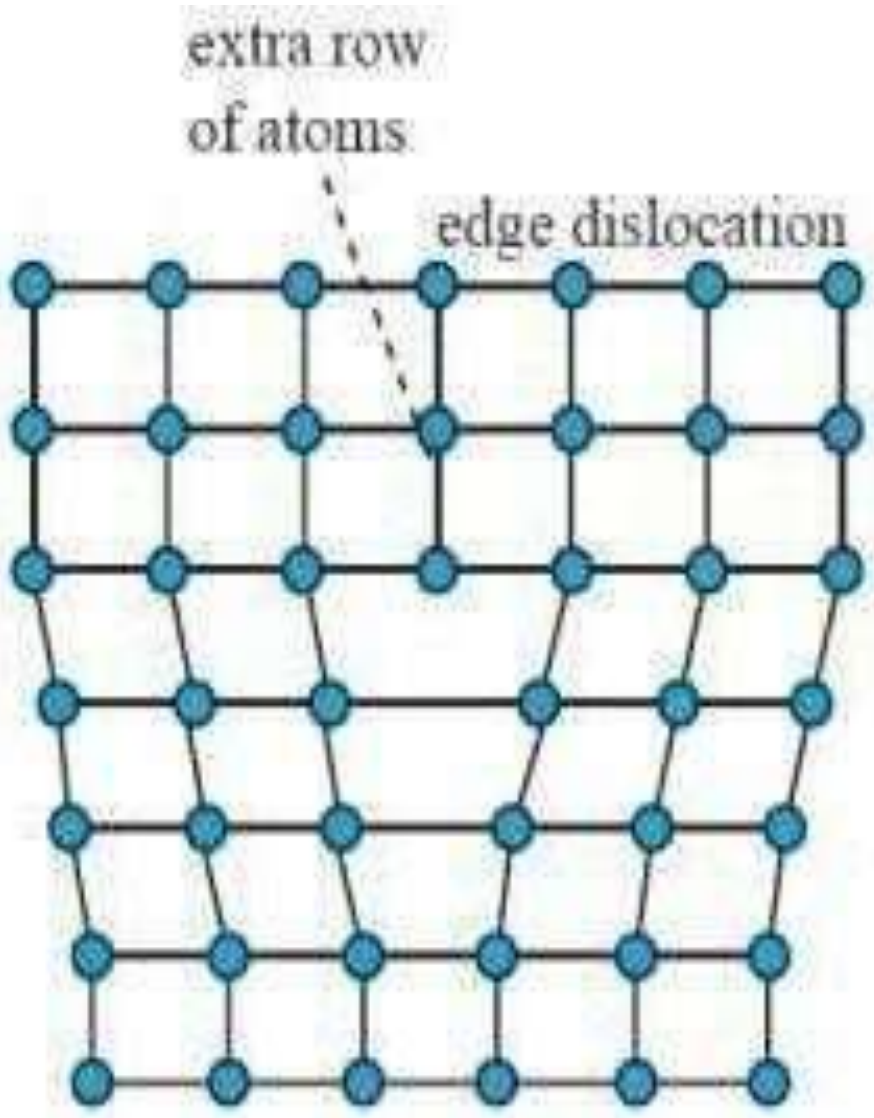
(b) Frenkel defect

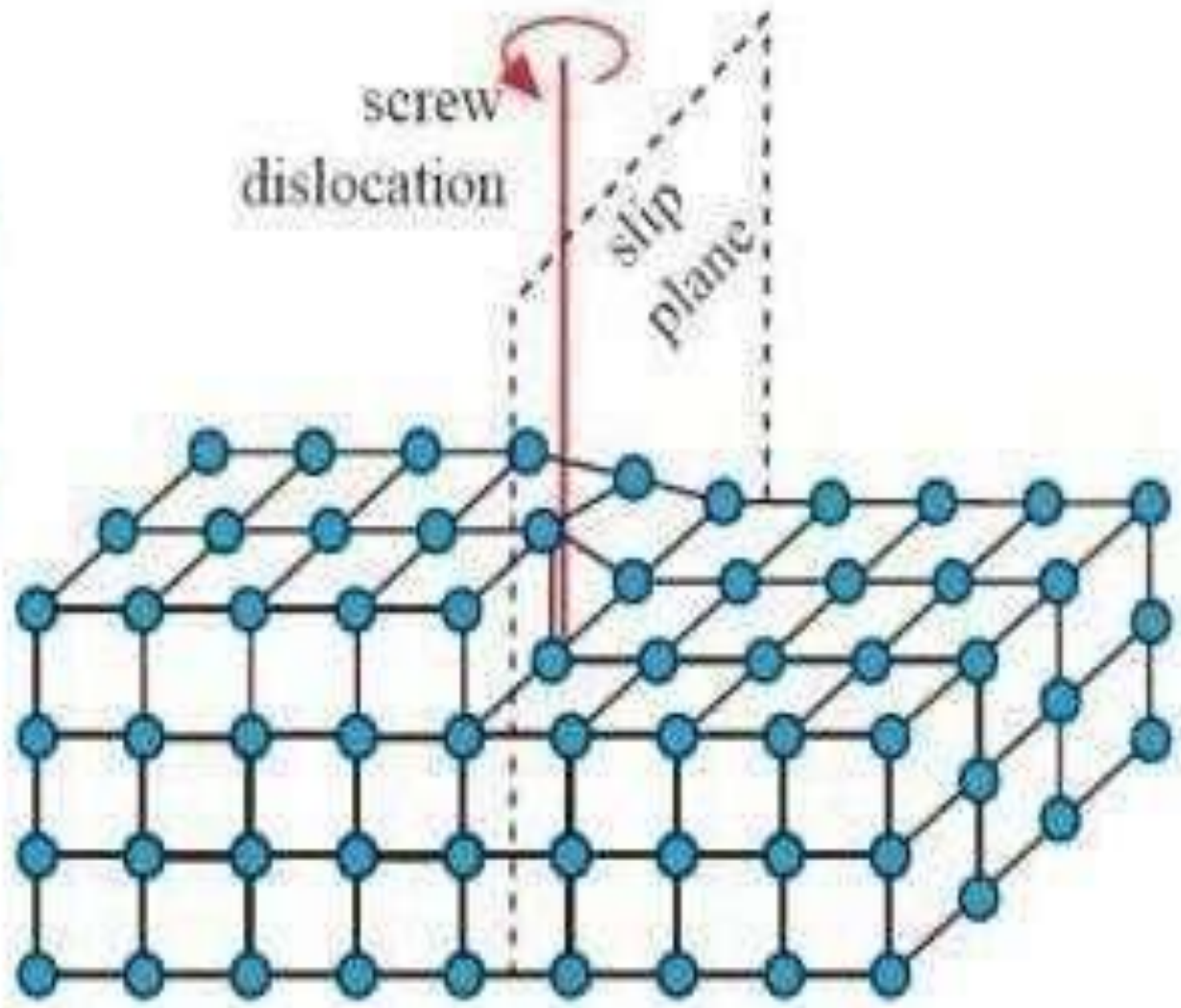
LINE DEFECTS

- Line defects are the irregularities or deviations from ideal arrangement in entire rows of lattice points.



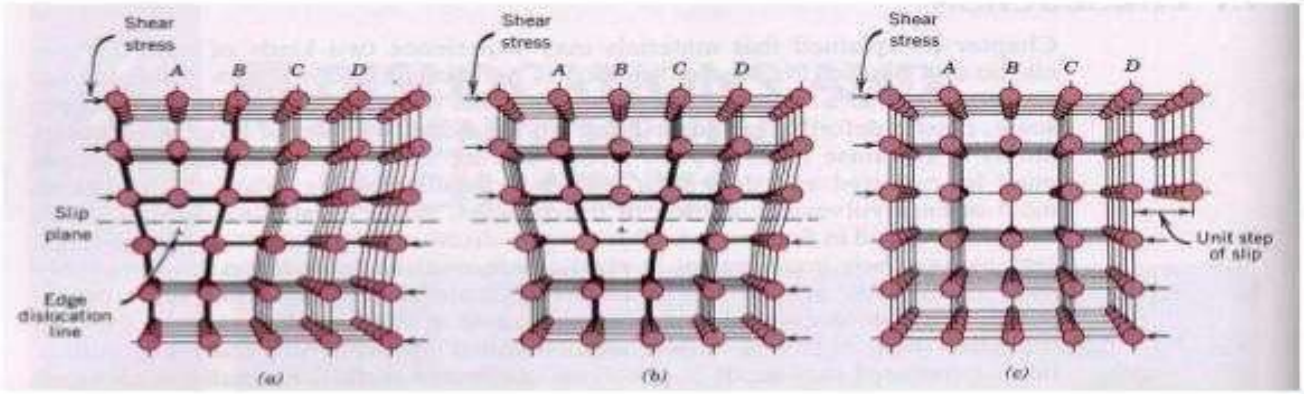
- Interatomic bonds significantly distorted in immediate vicinity of dislocation line.
- Dislocation affects the mechanical properties.


extra row
of atoms
edge dislocation

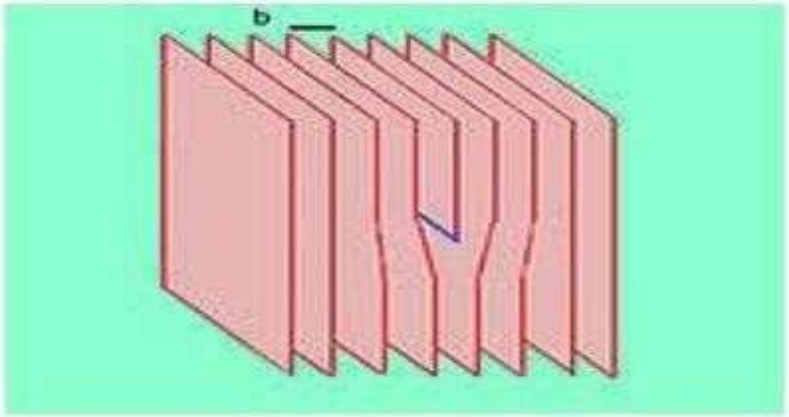

screw
dislocation
slip
plane

Edge Dislocation

- **The figure shows shear force is applied on its upper and lower surfaces.**
- **Consequently an extra half plane is introduced.**
- **Due to this extra half plane the crystal is badly distorted.**

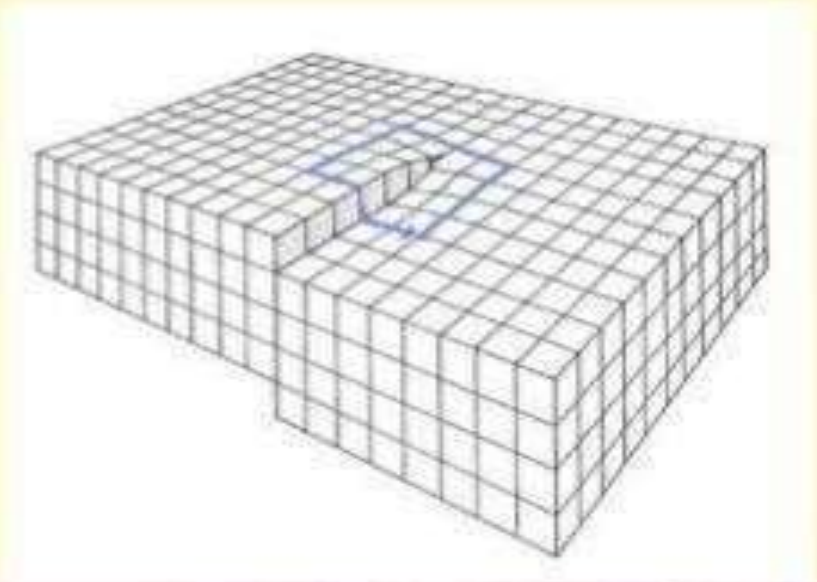


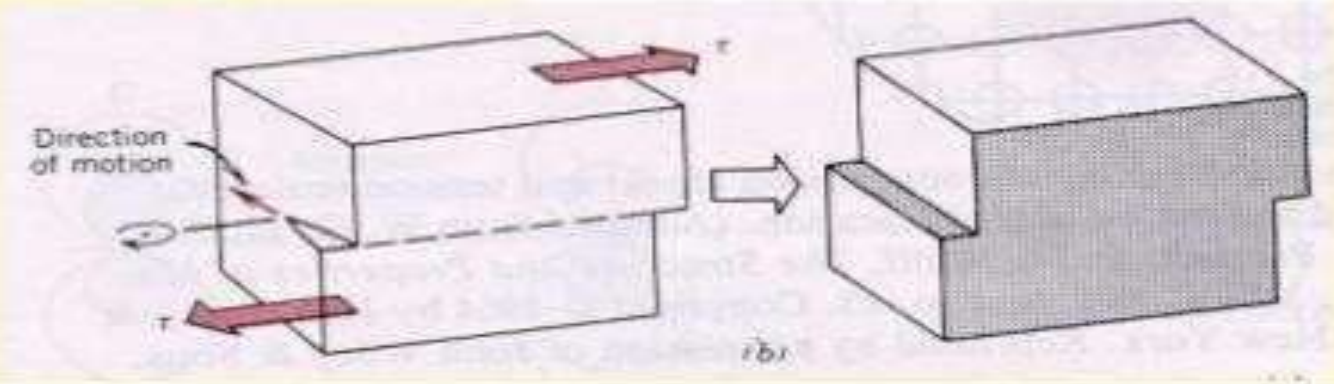
An edge dislocation is a defect where an extra half-plane of atoms is introduced mid way through the crystal.



Screw dislocation

- A dislocation in the lattice structure of a crystal in which the atoms are arranged in a helical pattern that is normal to the direction of the stress
- The motion of screw dislocation is also a result of shear stress
- Motion is perpendicular to direction of stress

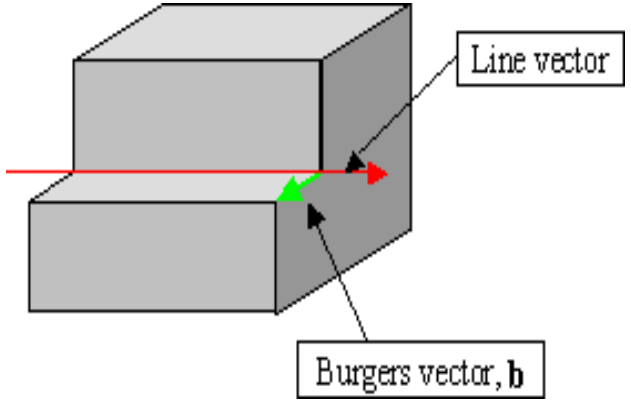




Edge vs Screw Dislocation

More Information Online WWW.DIFFERENCEBETWEEN.COM

	Edge Dislocation	Screw Dislocation
DEFINITION	A form of a line defect in crystal lattices in which the defect occurs either due to the presence of an extra plane of atoms or due to the loss of a half of a plane of atoms in the middle of the lattice	A form of a line defect in which the defect occurs when the planes of atoms in the crystal lattice trace a helical path around the dislocation line
OUTCOME OF GRAMS STAINING	When we apply stress on a crystal having edge dislocation, the dislocation area moves parallel to the direction of stress	When we apply stress on a crystal having this defect, the dislocation area moves perpendicular to the direction of stress
STRESS	Stress is comparatively less complex	Stress is comparatively complex



Comparison

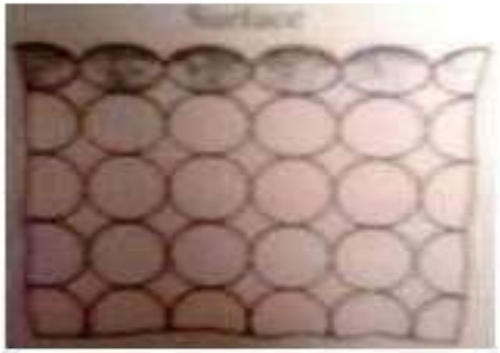
Edge Dislocation	Screw Dislocation
Arise due to introduction or elimination of an extra row of atoms	Arise due to partial slipping of section of crystal plane, where planes of atoms are transformed into surface of helix of screw
Tensile, compressive or shear stress field may be present	Only shear stress field is present
Lattice disturbance extends along an edge inside crystal	Lattice disturbance extends into two separate planes at right angles to each other
Burger's vector is always perpendicular to dislocation line	Burger's vector is parallel to dislocation line
Dislocations can climb and glide	Dislocation can only glide
Force required is less as compared to that for screw dislocation	Force required is more as compared to that of edge dislocation

SURFACE DEFECTS

- Surface defects are associated with boundaries that are separate regions of the materials and have different crystal structure.
- Two Dimensional defect.
- Due to change in orientation of the atomic planes and stacking sequence of atomic planes.
- Caused during solidification or mechanical or thermal treatment of material.
- Effect the mechanical properties, electrical resistance and corrosion resistance.

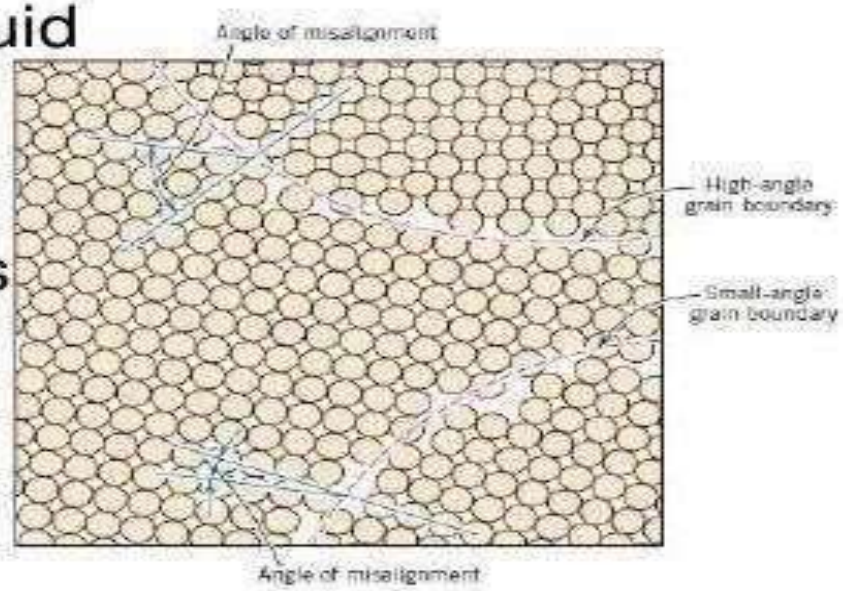
Surface Defects

1.External Surface:



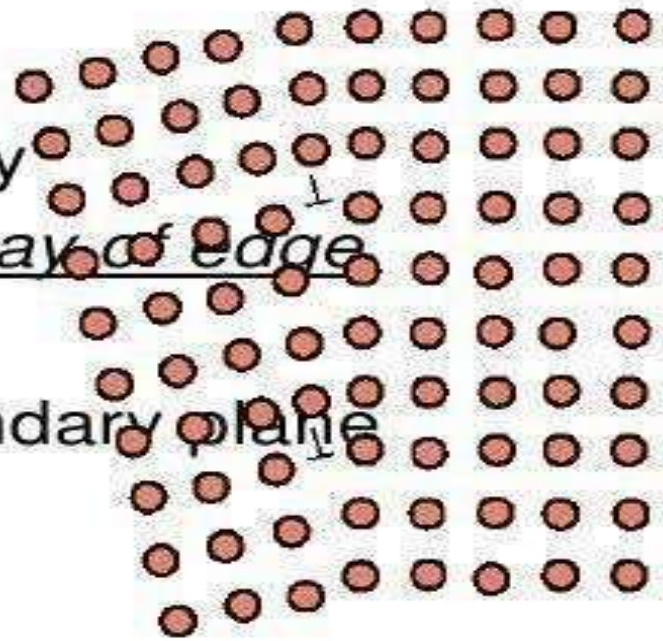
- Surface atoms have **unsatisfied atomic bonds,** and higher surface energies, than the bulk atoms.
- To reduce surface free energy, material tends to minimize its surface areas against the surface tension (e.g. liquid drop).

2.Grain boundaries:



- regions between two adjacent grains
- slightly disordered
- low density in grain boundaries
  - high mobility
  - high diffusivity
  - high chemical reactivity

3.Tilt Boundary:



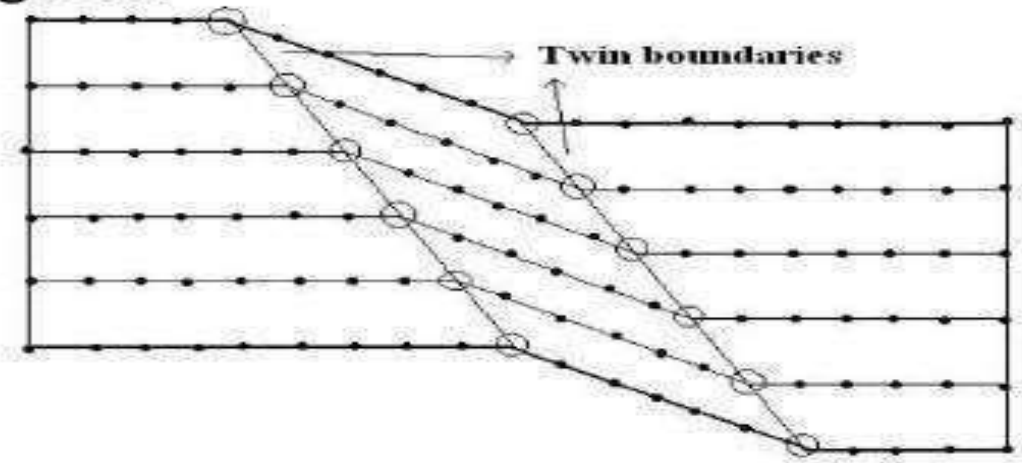
- A Tilt Boundary, between two slightly mis-aligned grains appears as an *array of edge dislocations*.
- Rotation axis is parallel to the boundary plane

4. Twist Boundary:

- Rotation axis is perpendicular to the boundary plane
- Low angle grain boundaries, that appear as *an array of Screw dislocations.*

5.Twin boundaries:

- These are the boundaries in the grains at which the atomic arrangement on one side of the boundary is the mirror image of the atoms on the other side .
- May be produced by shear deformation.
- The region between the pair of boundaries is called the twinned region.



6.Stacking Faults:

- Formed by fault in the stacking sequence of atomic planes in crystals.
- Considering stacking arrangement in FCC:

ABCABCABCABCABCABC

ABCABC BCABCABC

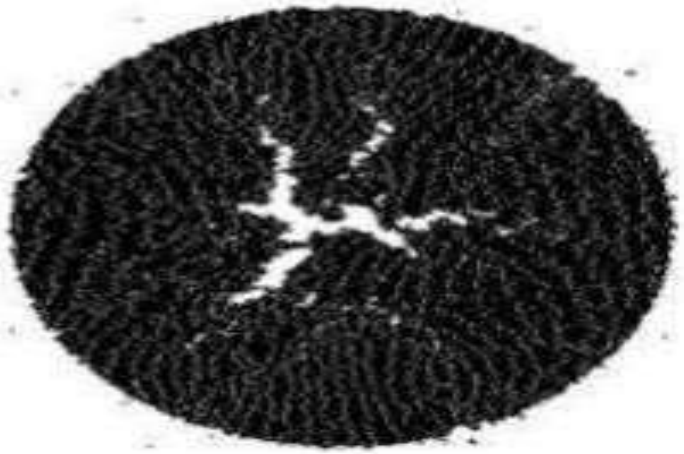
- This thin region is a surface imperfection and is called Stacking faults.

3.5. Volume defects

- Volume defects are two-dimensional defects
- Volume defects such as cracks may arise in crystals during the process of crystal growth.
- While growing, any possible small electrostatic dissimilarity between the stacking layers may result in crack.

Bulk or Volume Defects

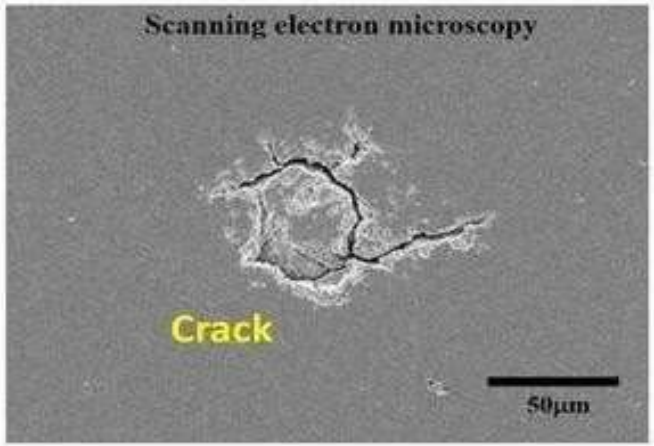
- **PERCIPITATES** : Fraction of a micron in size
- **DISPERSANTS** : may be large precipitates, grains, or polygranular particles distributed through microstructure
- **INCLUSIONS** : foreign particles or large precipitate particles ; undesirable ; harmful
- **VOIDS** : Trapped Gases ; Decreases mechanical strength

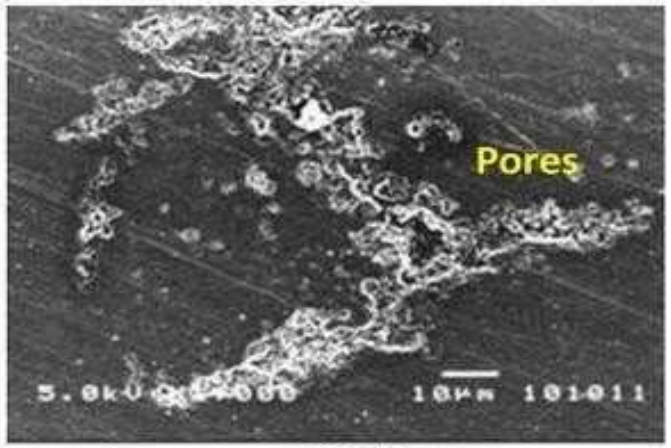


Cluster of microcracks in a melanin granule irradiated by a short laser pulse.

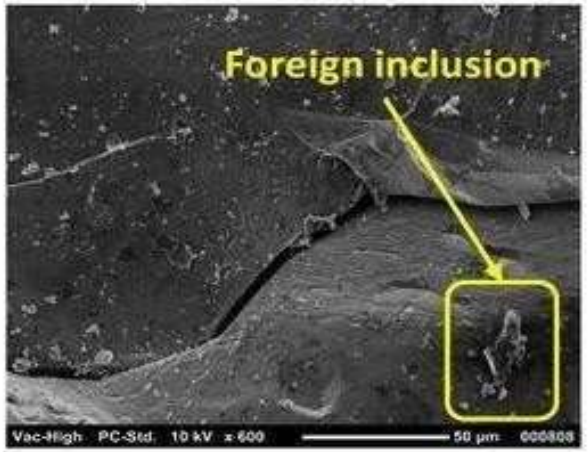
Volume Defects

- Volume defects include pores, cracks, foreign inclusions and other phases.
  - Pores : Affect optical, thermal and mechanical properties
  - Cracks : Affect mechanical properties
  - Foreign inclusion: Affect electrical, optical and mechanical properties
- Normally occurs during processing and fabrication processes.

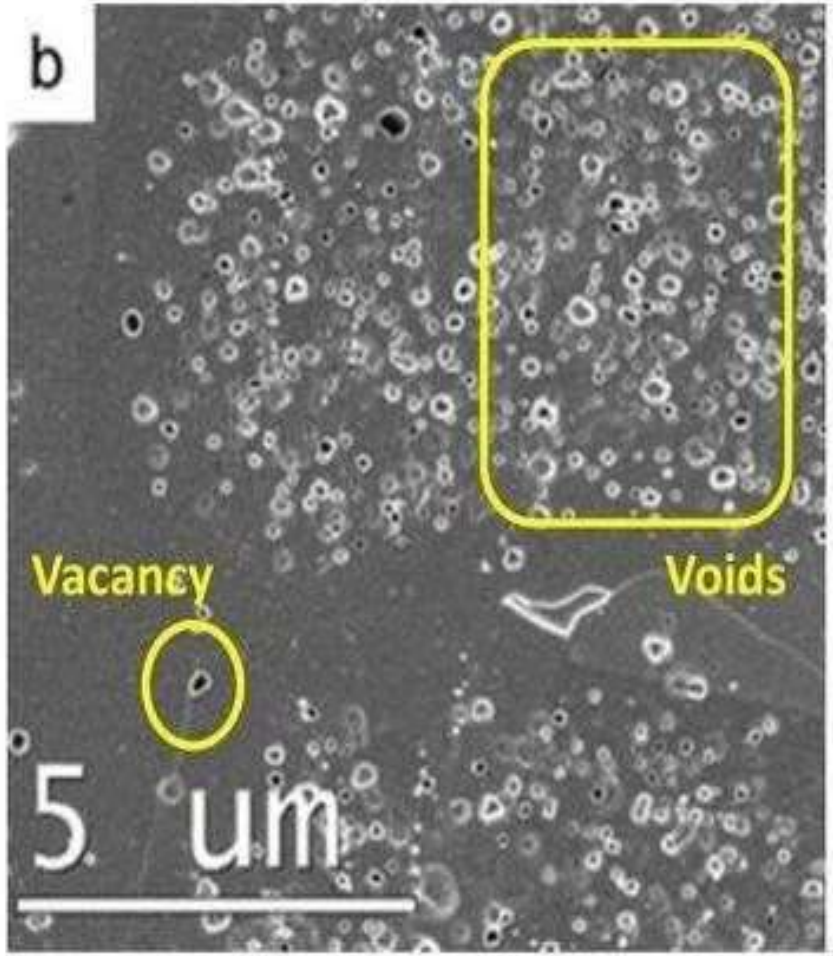




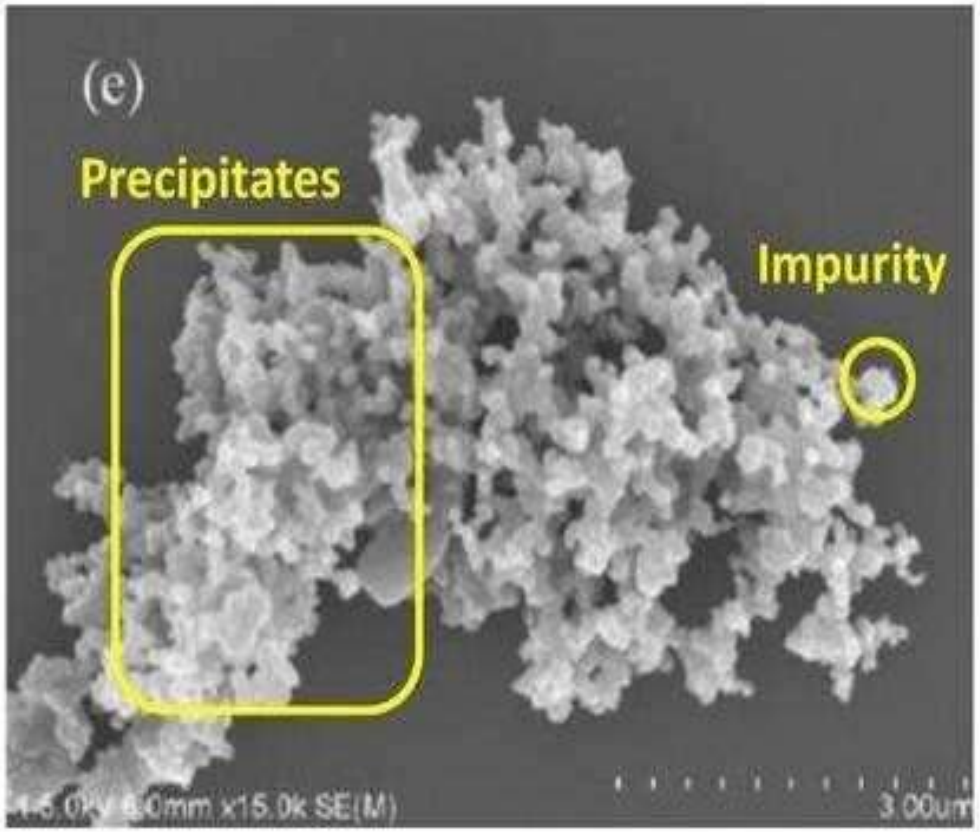
(b) 10 μm



Voids : Combination of several vacancies cause cluster void.

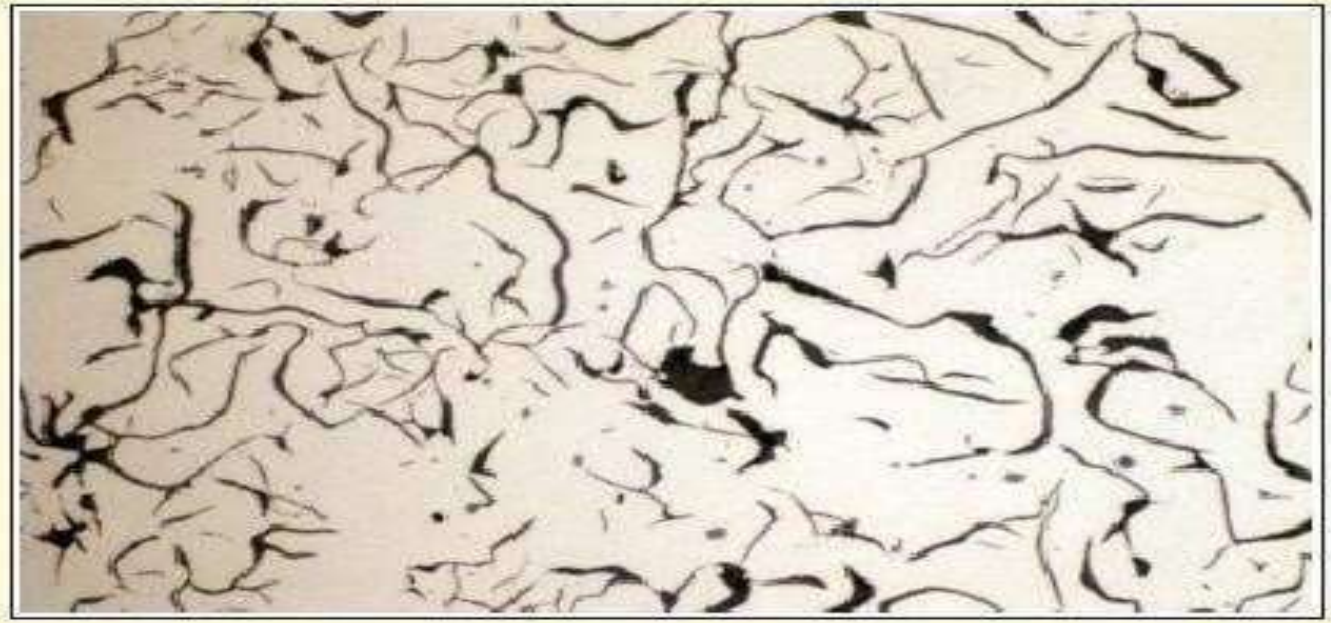


Precipitates : Combination of impurities to form small region of different phase.



Precipitates defect

- Second phase in solid. Can be void, gas bubble, or another solid.
- When insoluble foreign particles are present in a melt, these may be trapped in the solid during solidification.
- If the impurity is soluble in the solid at the melting point, it may precipitate out as the solid is cooled. (Solid solubility normally decreases as temperature is decreased.) These precipitates may be gas bubbles, impurity itself, or compound between impurity and solid.
- Example: carbon flakes in gray cast iron:
- Other methods of forming composite materials:
- Mixing of concrete and then hardening by formation of hydrate crytals.
- Mixing of fibers with a monomer and then polymerizing.



http://www.metallographic.com/Technical/Metallography-Intro.html

Mechanism of Strengthening in Metals

- The ability of a metal to plastically deform depends on the ability of dislocations to move.
- Hardness and strength are related to the ease with which plastic deformation can be made to occur
  - To enhance mechanical strength ➔ reduce dislocation mobility ➔ greater mechanical forces required to initiate plastic deformation.
- Strengthening mechanism for single phase metal
  - By grain size reduction
  - Solid-solution alloying
  - Strain-hardening

Mechanisms of strengthening in metals

- The ability of a metal to plastically deform depends on the ability of dislocations to move.
- ductility is sacrificed when an alloy is strengthened
- restricting or hindering dislocation motion renders a material harder and stronger.

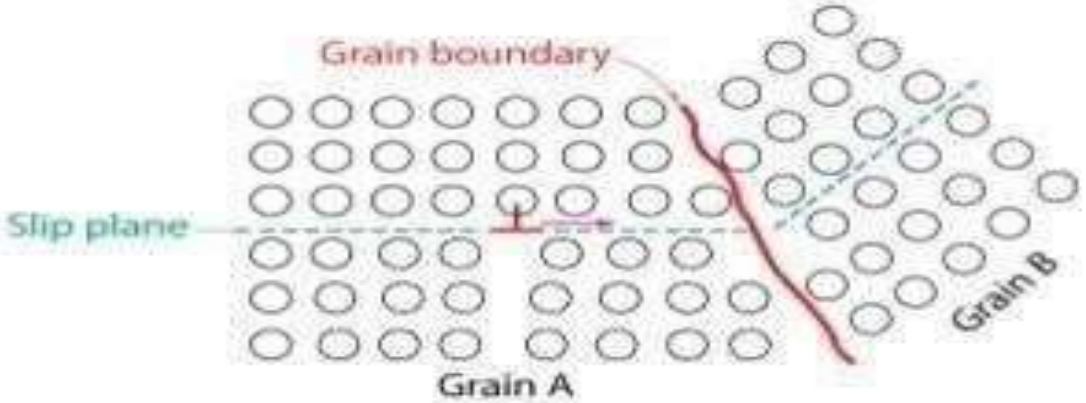
- strengthening mechanisms for single phase metals, by grain size reduction, solid-solution alloying, and strain hardening(cold work).

Strengthening by Grain size reduction

Grain boundaries are barriers to slip.

- Barrier "strength" increases with Increasing angle of misorientation.
- Smaller grain size: more barriers to slip

It is based on the fact that dislocations will experience hindrances while trying to move from a grain into the next because of abrupt change in orientation of planes.



Yield strength is related to grain size (diameter, d) as *Hall-Petch relation:*

$$\sigma_y = \sigma_i + kd^{-1/2}$$

Adapted from Fig. 7.14, *Callister 7e.* (Fig. 7.14 is from *A Textbook of Materials Technology*, by Van Vlack, Pearson Education, Inc., Upper Saddle River, NJ.)

Strengthening by Grain size reduction (Contd...)

Grain Size Reduction Techniques:

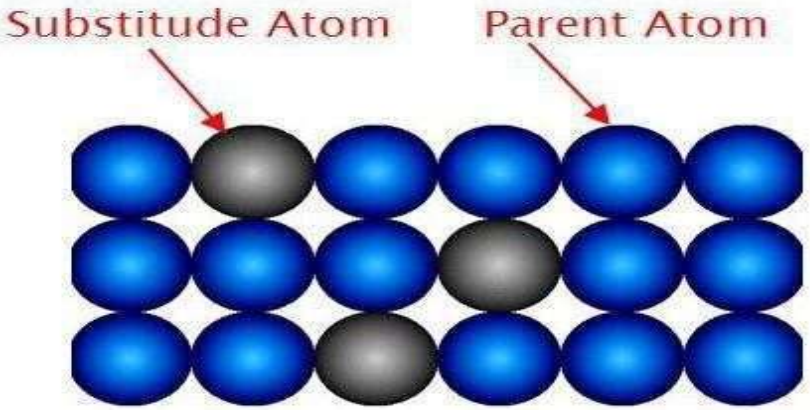
- Increase Rate of solidification from the liquid phase.
- Perform Plastic deformation followed by an appropriate heat treatment.

Notes:

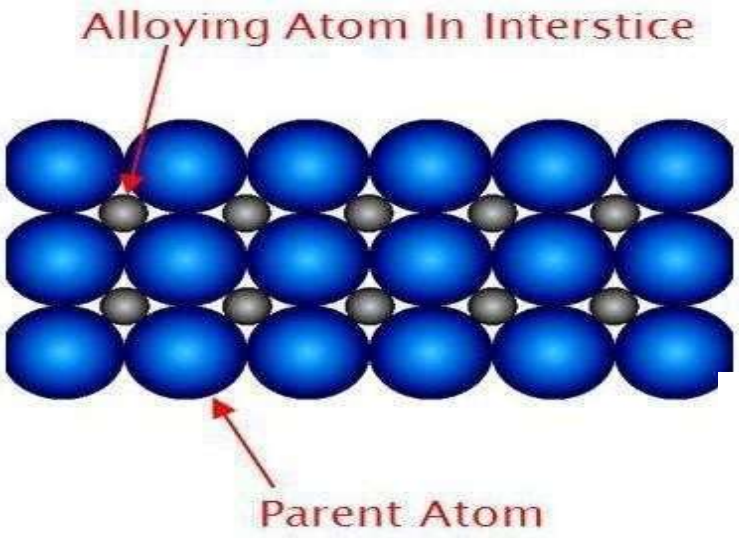
- Grain size reduction also improves toughness of many alloys.
- Small-angle grain boundaries are not effective in interfering with the slip process because of the small crystallographic misalignment across the boundary.
- Boundaries between two different phases are also impediments to movements of dislocations.

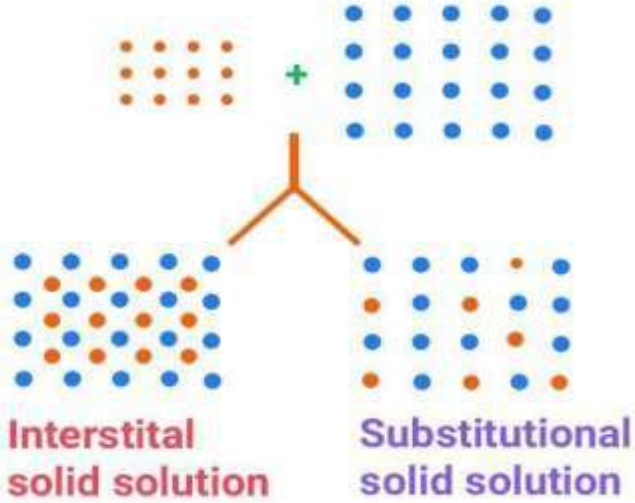
2 Types of Solid Solutions

Substitutional Solid Solution Alloys



Interstitial Solid Solution Alloys

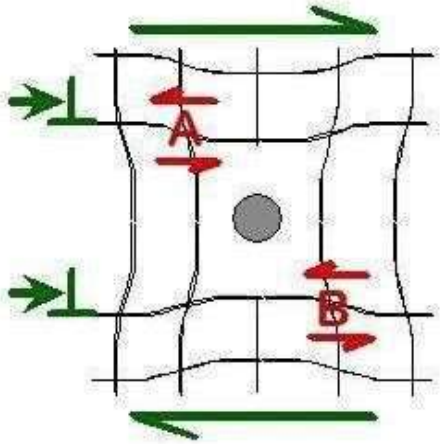




Solid-solutions strengthening

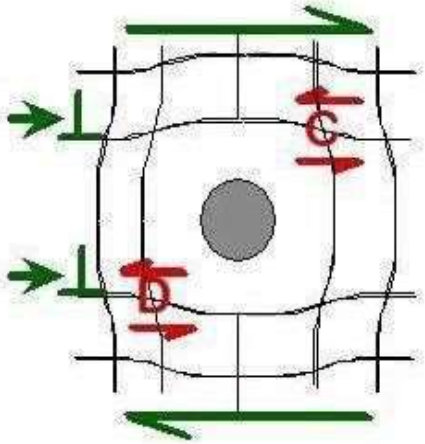
- Impurity atoms distort the lattice & generate stress
- Stress can produce a barrier to dislocation motion

Smaller substitutional impurity

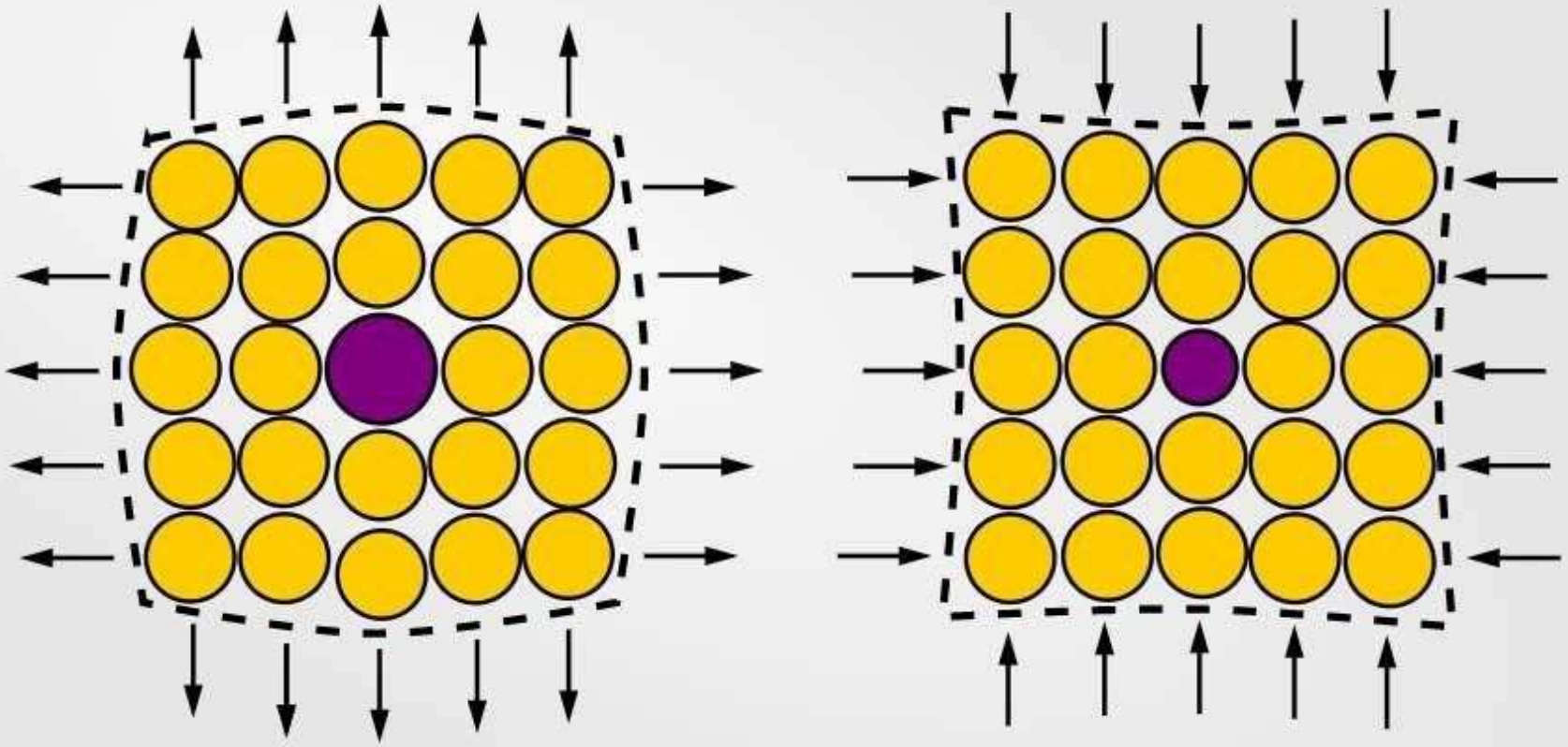


Impurity generates local shear at A and B that opposes dislocation motion to the right.

Larger substitutional impurity



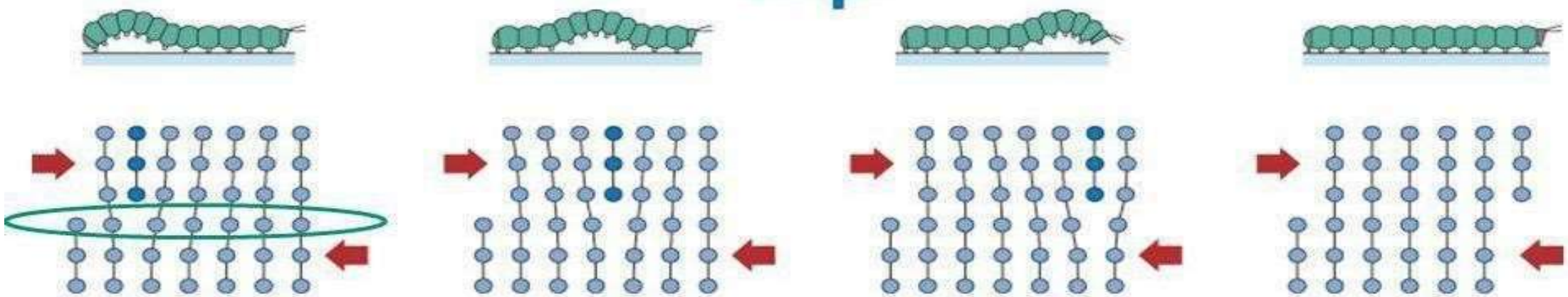
Local Stress in Substitutional Solid Solution



Dislocation and slip

- In materials science, a **dislocation** or Taylor's **dislocation** is a linear crystallographic defect or irregularity within a crystal structure that contains an abrupt change in the arrangement of atoms.
- The movement of **dislocations** allow atoms to slide over each other at low stress levels and is known as glide or **slip**.

Slip



- The process by which plastic deformation is produced by dislocation motion is called **slip (movement of dislocations)**.
- The extra ½-plane moves along the slip plane.
- Dislocation movement is similar to the way a caterpillar moves. The caterpillar hump is representative of the extra ½-plane of atoms.

Critical Resolved Shear Stress (CRSS)

Critical resolved shear stress is the component of SHEAR STRESS, resolved in the direction of slip, necessary to initiate slip in a grain.

It is a constant for a given CRYSTAL.

Tests have been conducted on single crystals of metals to measure the shear stress required to initiate plastic deformation, or cause atomic planes to slip.

Since this is a threshold value, it is referred to as critical; and since it is a component of the applied force or stress, it is said to be resolved; that is, the ***critical resolved shear stress***.

Critical Resolved Shear Stress

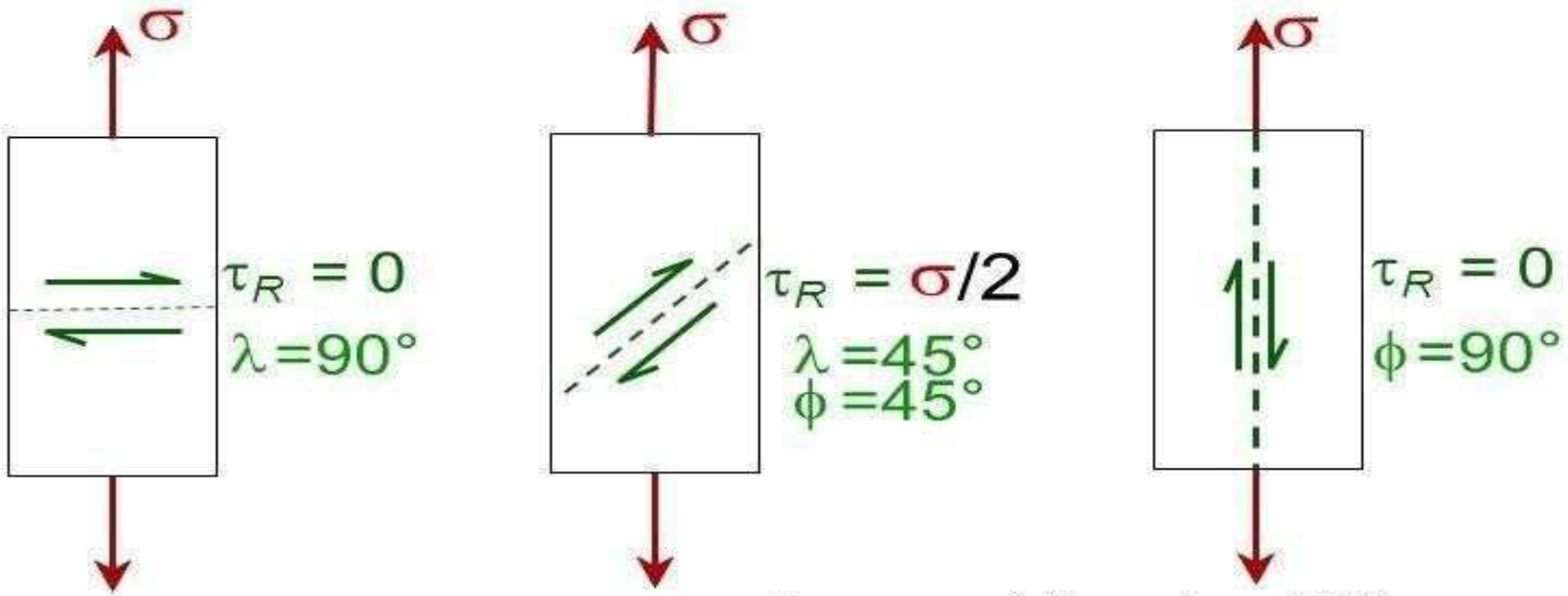
- Condition for dislocation motion: $\tau_{R\,(max)} > \tau_{CRSS}$

typically 10^{-4} GPa to 10^{-2} GPa

Critical resolved shear stress: is the minimum shear stress required to initiate slip and is a property of the material that determine when yielding occurs

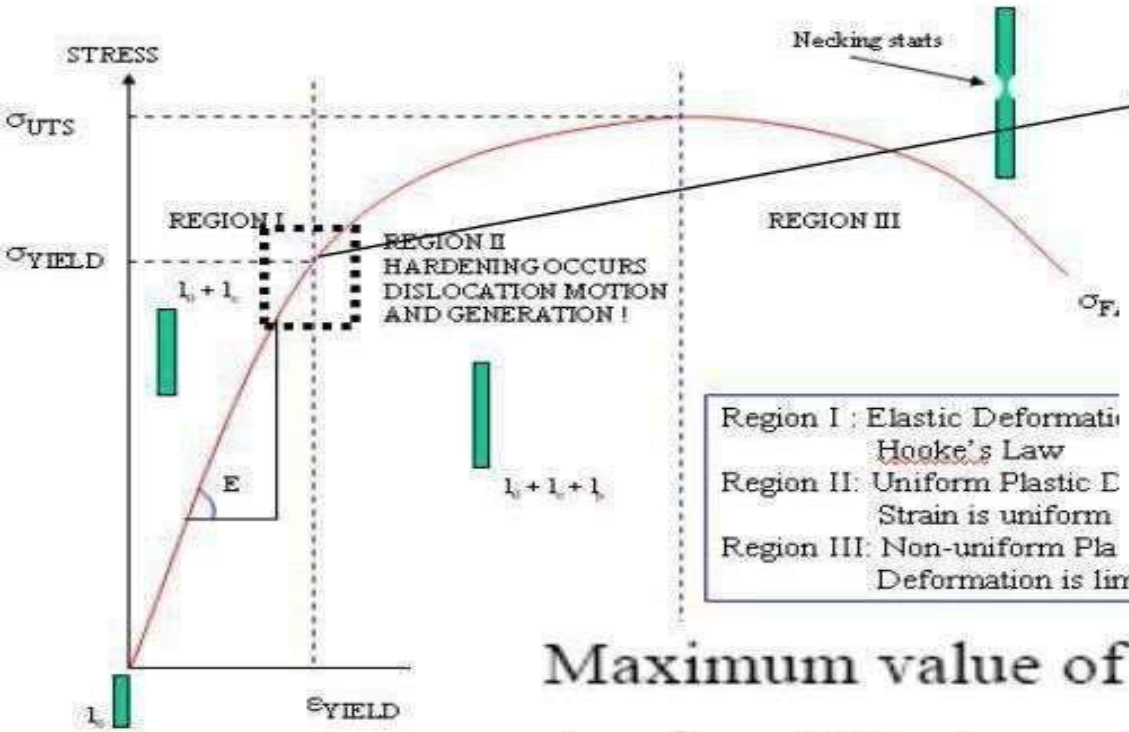
- Crystal orientation can make it easy or hard to move dislocation

$$\tau_R = \sigma \cos\lambda \cos\phi$$



τ maximum at $\lambda = \phi = 45°$

The Critical Resolved Shear Stress



Region I : Elastic Deformati
Hooke's Law
Region II: Uniform Plastic D
Strain is uniform
Region III: Non-uniform Pla
Deformation is limited to "neck" region

The minimum shear stress required to initiate slip is termed:
the critical resolved shear stress

$$\tau_{CRSS} = \sigma_y (\cos\phi \cos\lambda)_{MAX}$$

$$\sigma_y = \frac{\tau_{CRSS}}{(\cos\phi \cos\lambda)_{MAX}}$$

Maximum value of ($\cos\phi \cos\lambda$) corresponds to

$$\phi = \lambda = 45° \Rightarrow \cos\phi \cos\lambda = 0.5 \Rightarrow \sigma_y = 2\tau_{CRSS}$$

Slip will occur first in slip systems oriented close to this angle ($\phi = \lambda = 45°$) with respect to the applied stress

What is an alloy?

- Alloy is a mixture of two or more elements having metallic properties.
- The element present in the largest portion is a metal and others can be metals or non-metals
- The element which is present in the largest amount is called as the **base metal** or **parent metal** or **solvent**
- Other alloying elements are called as **solute**

"An **alloy** is a mixture of two elements, one of which is a **metal**. **Alloys** often have properties that are different to the **metals** they contain. This makes them more useful **than** the **pure metals** alone. For example, **alloys** are often harder **than** the **metal** they contain."

Necessity of Alloying

- Pure metals possess few important physical and metallic properties, such as melting point, boiling point, density, specific gravity, high malleability, ductility, and heat and electrical conductivity.
- These properties can be modified and enhanced by alloying it with some other metal or nonmetal, according to the need
- Alloys are made to:

- Enhance the hardness of a metal

An alloy is harder than its components. Pure metals are generally soft. The hardness of a metal can be enhanced by alloying it with another metal or nonmetal.

EX: Bronze (Cu+ 11% tin) is harder than copper, making it useful for tools and weapons

❑Lower the melting point

Pure metals have a high melting point. The melting point lowers when pure metals are alloyed with other metals or nonmetals.

This makes the metals easily fusible. This property is utilized to make useful alloys called solders.

EX:

Tin, lead and their alloys, due to their low melting temperatures and wide availability, are the most commonly used solder materials

- **Enhance tensile strength**

  Alloy formation increases the tensile strength of the parent metal

- **Enhance corrosion resistance**

  Alloys are more resistant to corrosion than pure metals. Metals in pure form are chemically reactive and can be easily corroded by the surrounding atmospheric gases and moisture. Alloying a metal increases the inertness of the metal, which, in turn, increases corrosion resistance.

  EX:

  Stainless Steel (alloy of Fe and Cr) is more corrosion resistant than Iron

- **Modify color**

  The color of pure metal can be modified by alloying it with other metals or nonmetals containing suitable color pigments

- **Provide better cast ability**

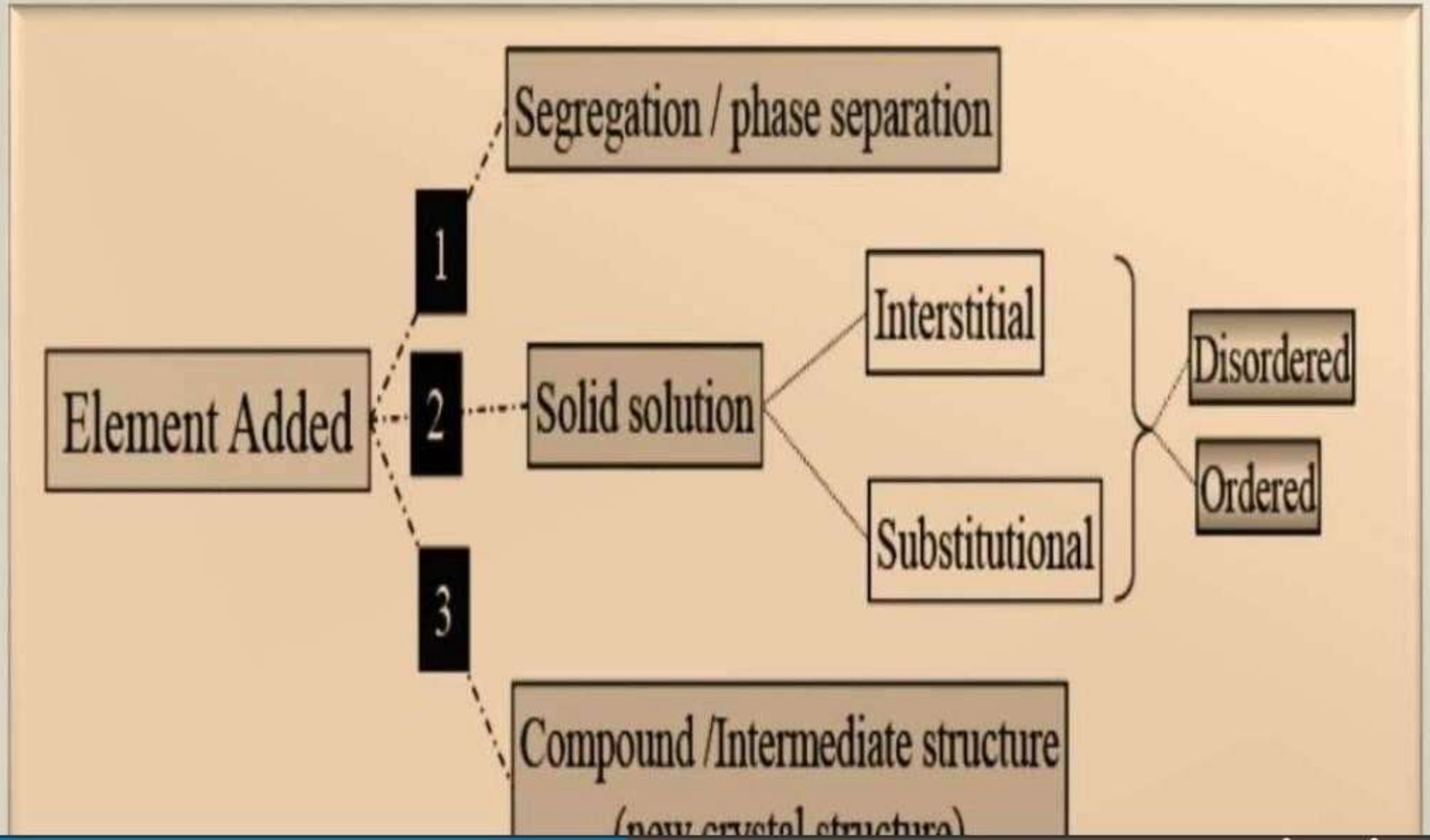
  One of the most essential requirements of getting good castings is the expansion of the metal on solidification.

  Pure molten metals undergo contraction on solidification. Metals need to be alloyed to obtain good castings because alloys expand

11 Examples of Alloys in Everyday Life

- https://studiousguy.com/examples-of-alloys/

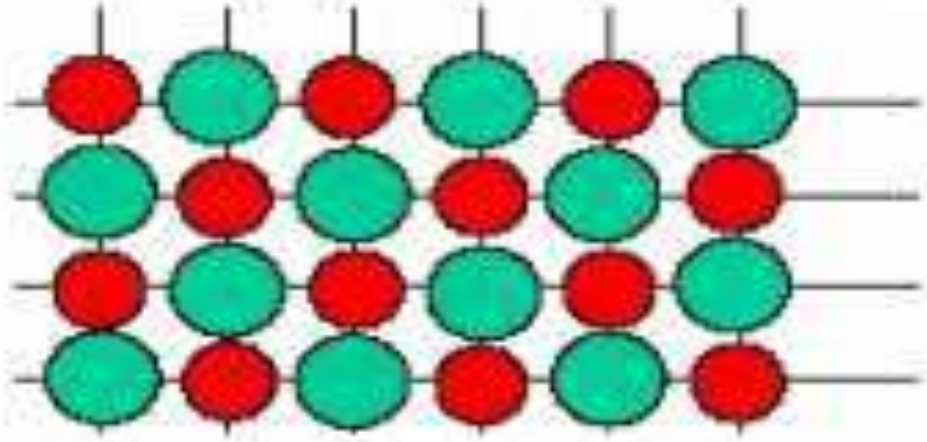
Classification of alloy systems



Ordered Substitutional and Interstititials Compounds

Substitutional

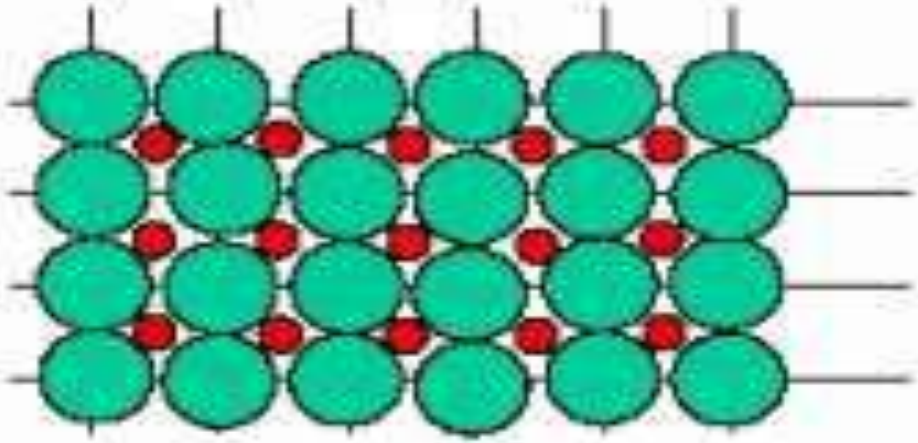
'an element replaces host atoms in an orderly arrangement'



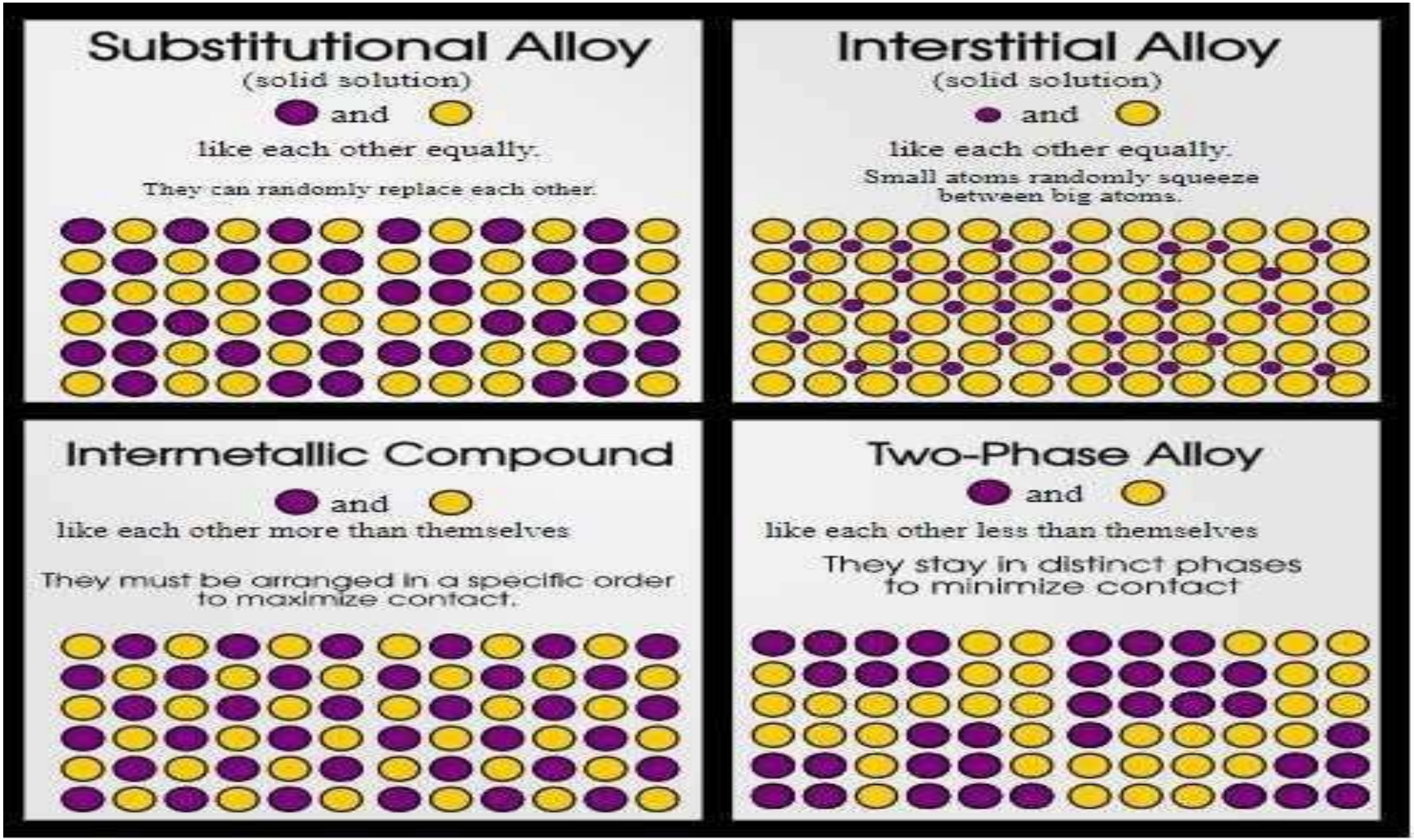
e.g., Ni_3Al (hi-T yield strength), $Al_3(Li,Zr)$ (strengthening)

Interstitial

'an element goes into holes in an orderly arrangement'



e.g., small impurities, clays ionic crystals, ceramics.


Substitutional Alloy
(solid solution)
and
like each other equally.
They can randomly replace each other.
Interstitial Alloy
(solid solution)
and
like each other equally.
Small atoms randomly squeeze between big atoms.
Intermetallic Compound
and
like each other more than themselves
They must be arranged in a specific order to maximize contact.
Two-Phase Alloy
and
like each other less than themselves
They stay in distinct phases to minimize contact

Properties of a Materials

Properties of a materials depend on

1. Number of phases present
2. Types of phases present
3. Amount of phases present and
4. Distribution of the phases present

The Properties can be changed by altering these quantities.

In order to make these changes, it is essential to know the conditions under which these quantities exist and the conditions under which a change in phase will occur.

Phase Diagram

- A **phase diagram** is a type of chart used to show conditions at which thermodynamically distinct phases can occur at equilibrium at different temperature, pressure and composition.
- **The best method to record the data related to phase changes in many alloy systems is in the form of *phase diagrams*, also known as *equilibrium diagrams* or *constitutional diagrams*.**

Phase diagrams

- **In order to specify completely the state of a system in equilibrium, it is necessary to specify three independent variables.**
- **These variables, which are externally controllable, are *temperature, pressure* and *composition*.**
- Phase diagram is the graphical presentation of the phases present in a system under different conditions of pressure, temperature and composition.

Components of a Phase Diagram

- Common components of a phase diagram are *lines of equilibrium* or *phase boundaries*, which refer to lines that mark conditions under which multiple phases can coexist at equilibrium. Phase transitions occur along lines of equilibrium.
- Triple points are points on phase diagrams where lines of equilibrium intersect. Triple points mark conditions at which three different phases can coexist. For example, the water phase diagram has a triple point corresponding to the single temperature and pressure at which solid, liquid, and gaseous water can coexist in a stable equilibrium.
- The solidus is the temperature below which the substance is stable in the solid state.
- The liquidus is the temperature above which the substance is stable in a liquid state. There may be a gap between the solidus and liquidus; within the gap, the substance consists as a mixture of solid and liquid (like a "slurry").[1]

Phase diagrams in Metallurgical Systems

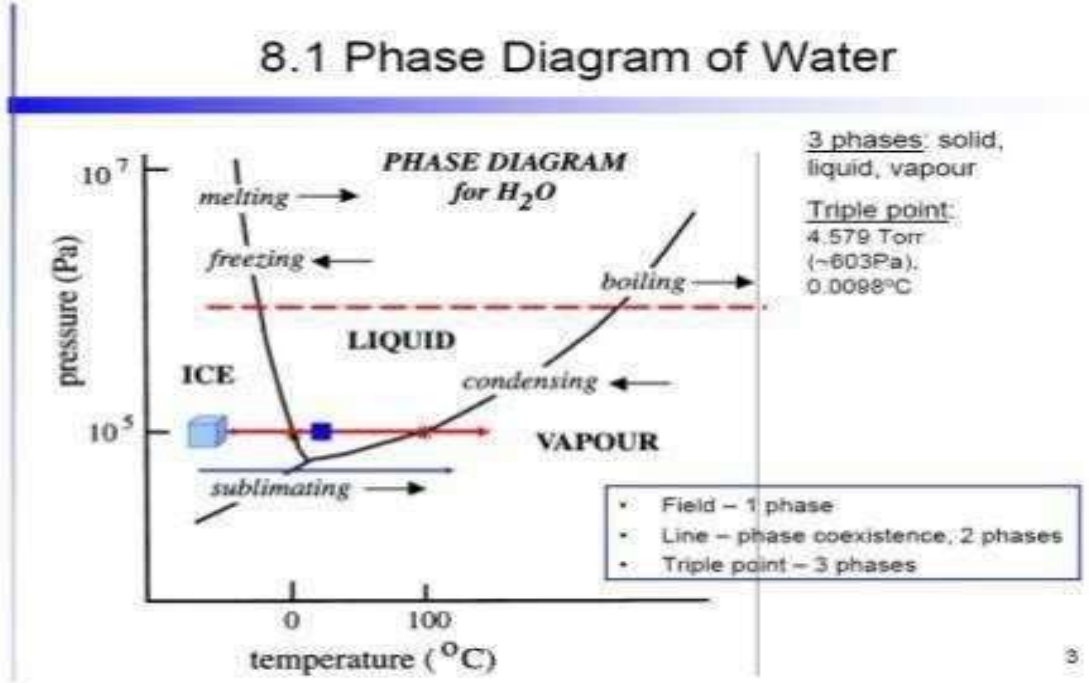
- In metallurgical systems, the pressure is usually taken as atmospheric pressure. Thus the phase diagram shows the phases present at different compositions and temperatures.
- **With pressure assumed to be constant at atmospheric pressure, the equilibrium diagram indicates the structural changes due to variation of temperature and composition.**
- **Phase diagrams show the phases present under equilibrium conditions, that is, under conditions in which there will be no change with time.**
- **Equilibrium conditions may be approached by extremely slow heating and cooling, so that if a phase change is to occur, sufficient time is allowed.**

Types of Phase Diagrams

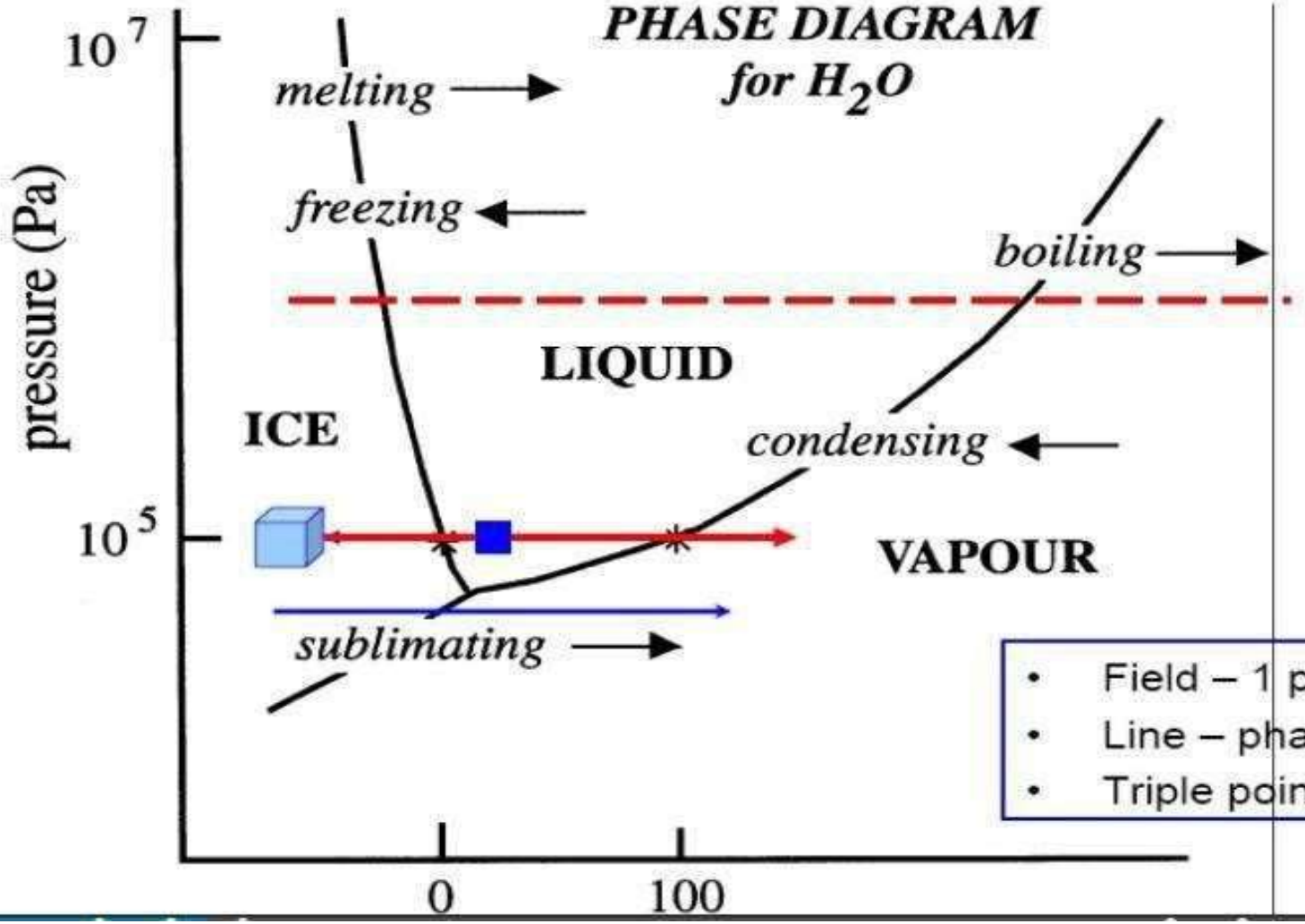
- The phase diagrams may be divided into the following three catagories
  - 1. Unary Phase Diagram
  - 2. Binary Phase Diagram
  - 3. Ternary Phase Diagram

A typical phase diagram for Water

- The simplest phase diagrams are pressure-temperature diagrams of a single simple substance, such as water.
- The axes correspond to the pressure and temperature.
- The phase diagram shows, in pressure-temperature space, the lines of equilibrium or phase boundaries between the three phases of solid, liquid, and gas.



8.1 Phase Diagram of Water



3 phases: solid, liquid, vapour

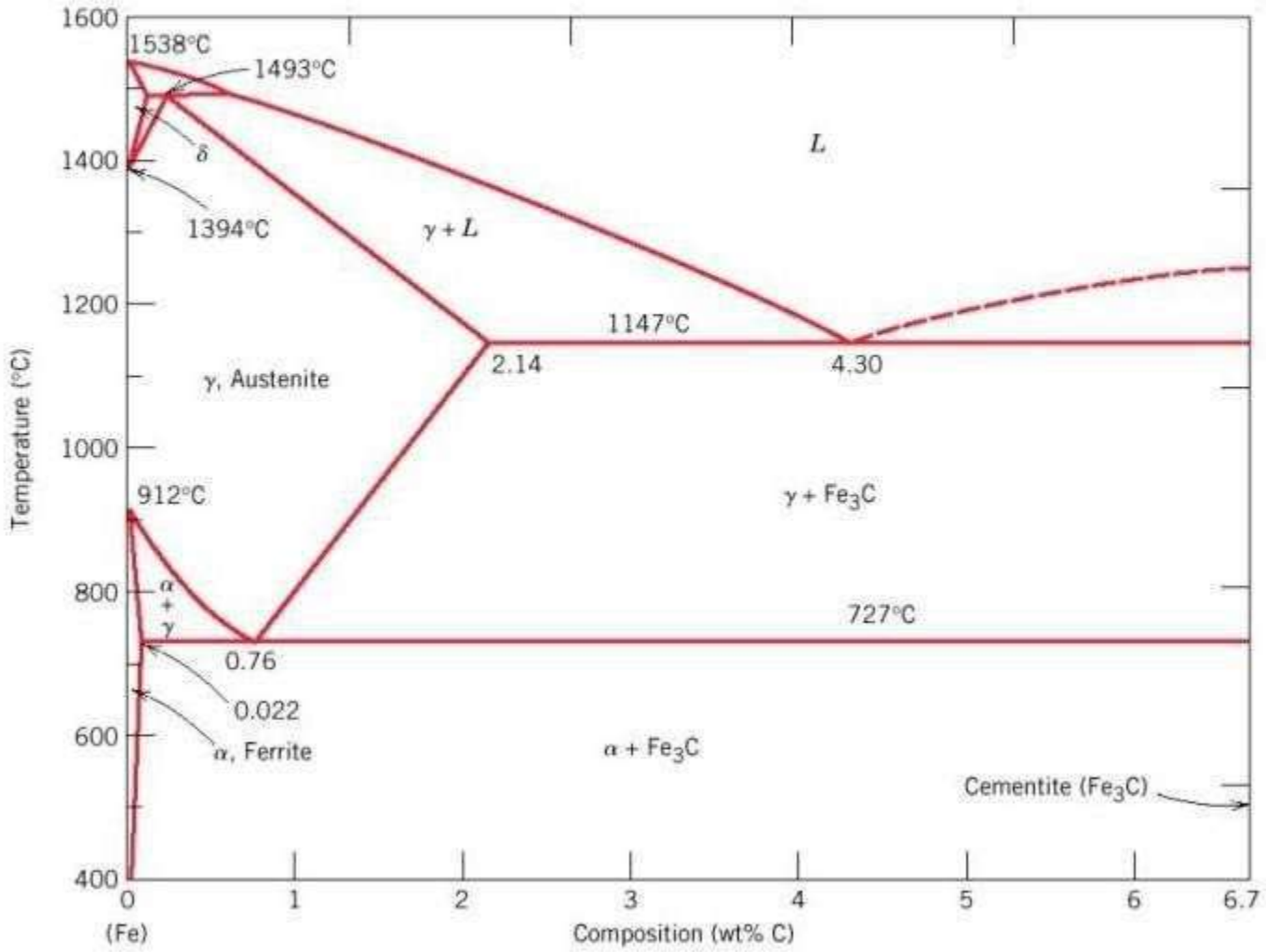
Triple point:
4.579 Torr
(~603Pa),
0.0098°C

- Field – 1 phase
- Line – phase coexistence, 2 phases
- Triple point – 3 phases

Iron–Carbon Phase Diagram

- In their simplest form, steels are alloys of Iron (Fe) and Carbon (C).
- The Fe-C phase diagram is a fairly complex one, but we will only consider the steel and cast iron part of the diagram, up to 6.67% Carbon.

Fe – C Equilibrium Diagram



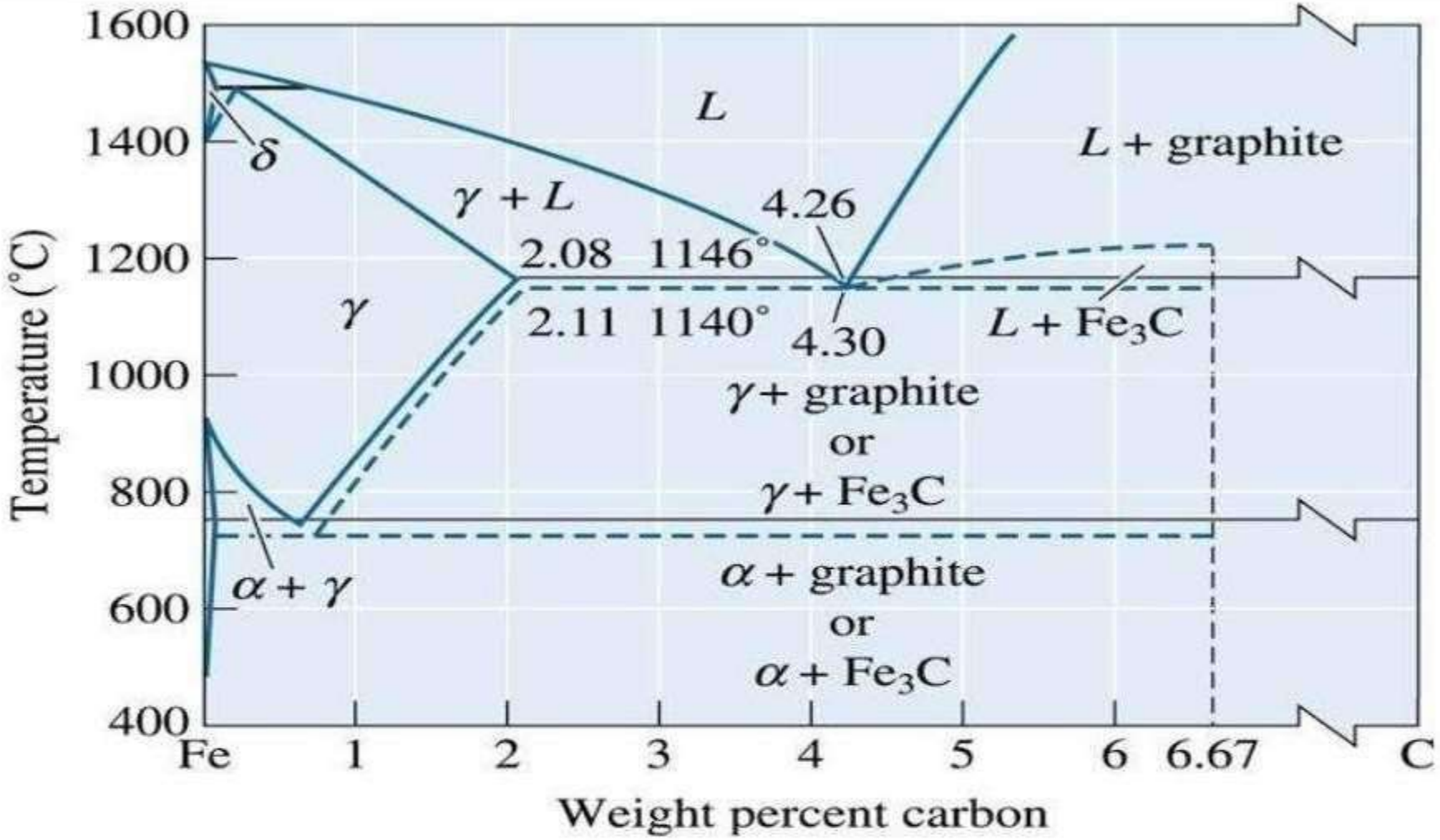


Figure 12.33 The iron-carbon phase diagram showing the relationship between the stable iron-graphite equilibria (solid lines) and the metastable iron-cementite reactions (dashed lines).

Phases Observed in Fe-C Diagram -

- Phases
    1. Ferrite
    2. Austenite
    3. Cementite
    4. δ-ferrite
- And phase mixtures
    1. Pearlite
    2. Ledeburite

Phases Observed in Fe-C Diagram

1. Ferrite

Ferrite is the interstitial solid solution of carbon in alpha iron. It has B.C.C. Structure. It has very limited solubility for carbon (maximum 0.022% at 727°C and 0.008% at room temperature). Ferrite is soft and ductile.

2. Austenite

Austenite is the interstitial solid solution of carbon in gamma (γ) iron. It has FCC structure. Austenite can have maximum 2.14% carbon at 1143°C. Austenite is normally not stable at room temperature. Austenite is non-magnetic and soft.

3. Cementite

Cementite or iron carbide (Fe_3C) is an intermetallic compound of iron and carbon. It contains 6.67% carbon. It is very hard and brittle. This intermetallic compound is a metastable phase and it remains as a compound indefinitely at room temperature.

4. δ-ferrite

It is a solid solution of carbon in δ-iron. It is stable at high temperatures. It has BCC structure.

Phase Mixtures Observed in Fe-C Diagram

- **1. Pearlite**

  The pearlite consists of alternate layers of ferrite and cementite. It has properties somewhere between ferrite and cementite. The average carbon content in pearlite is 0.76%

- **2. Ledeburite**

  Ledeburite is an eutetcic mixture of austenite and cementite in the form of alternate layers. The average carbon content in ledeburite is 4.3%.

A few comments on Fe–C system

- Carbon occupies interstitial positions in Fe. It forms a solid solution with α, γ, δ phases of iron
- Maximum solubility in BCC α-ferrite is limited (max. 0.025 % at 727 °C) as BCC has relatively small interstitial positions
- Maximum solubility in FCC austenite is 2.14 % at 1147 °C as FCC has larger interstitial positions

A few comments on Fe–C system

- Mechanical properties
  - Cementite is very hard and brittle - can strengthen steels.
  - Mechanical properties depend on the microstructure, that is, amount and distribution of ferrite and cementite.
- Magnetic properties: α -ferrite is magnetic below 768 °C, austenite is non-magnetic

Fe-C Alloys

- **Fe-C alloys can be of two types.**

1. Steels

Steels are alloys of iron and carbon containing up to 2.14% C. Other alloying elements may also be present in steels.

2. Cast irons

Cast irons are alloys of iron and carbon containing more than 2.14% C. Other alloying elements may also be present in cast irons.

Important Reactions in Fe-C System

- **There are three important reactions taking place in Fe-C system**

1. Eutectic reaction

2. Eutectoid reaction

3. Peritectic Reaction

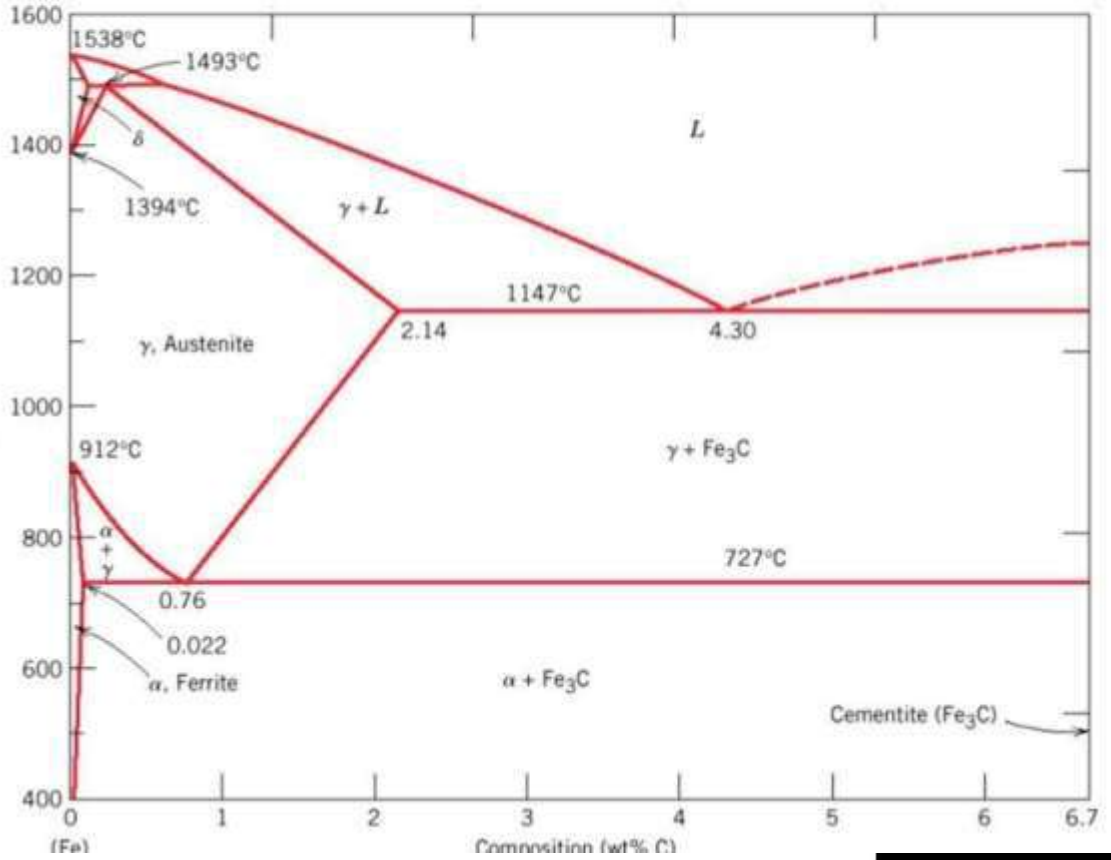
Important Reactions in Fe-C System

- Eutectic reaction
- **Eutectic: 4.30 wt% C, 1147 °C**
- **L (4.30% C) ↔ γ (2.14% C) + Fe_3C**

- Eutectoid reaction
- **Eutectoid: 0.76 wt%C, 727 °C**
- **γ(0.76% C) ↔ α (0.022% C) + Fe_3C**

- Peritectic Reaction
- **Peritectic: 0.16% C, 1493^0 C**
- **δ(0.11% C) + L(0.51%C) ↔ γ (0.16%C**

Fe – C Equilibrium Diagram

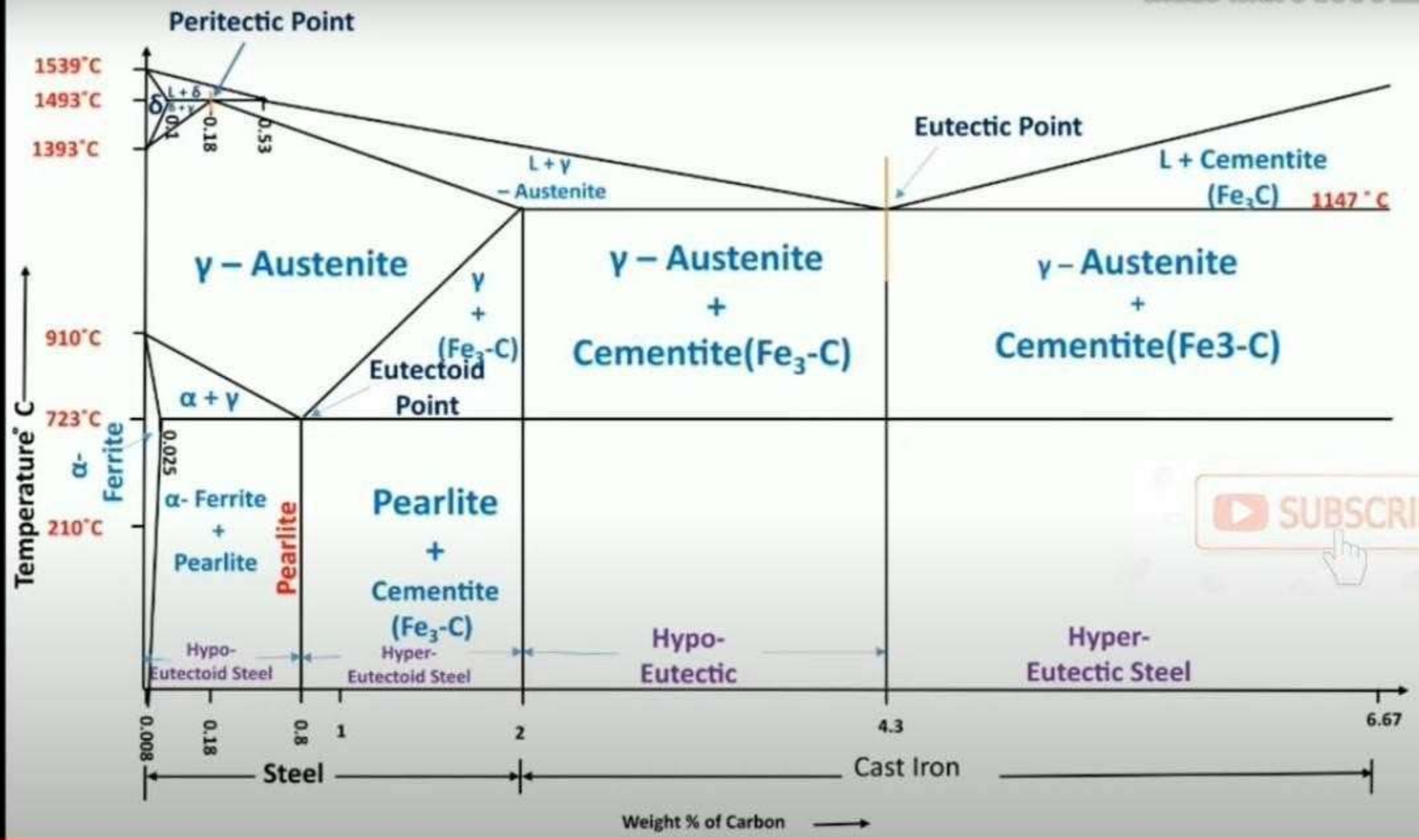


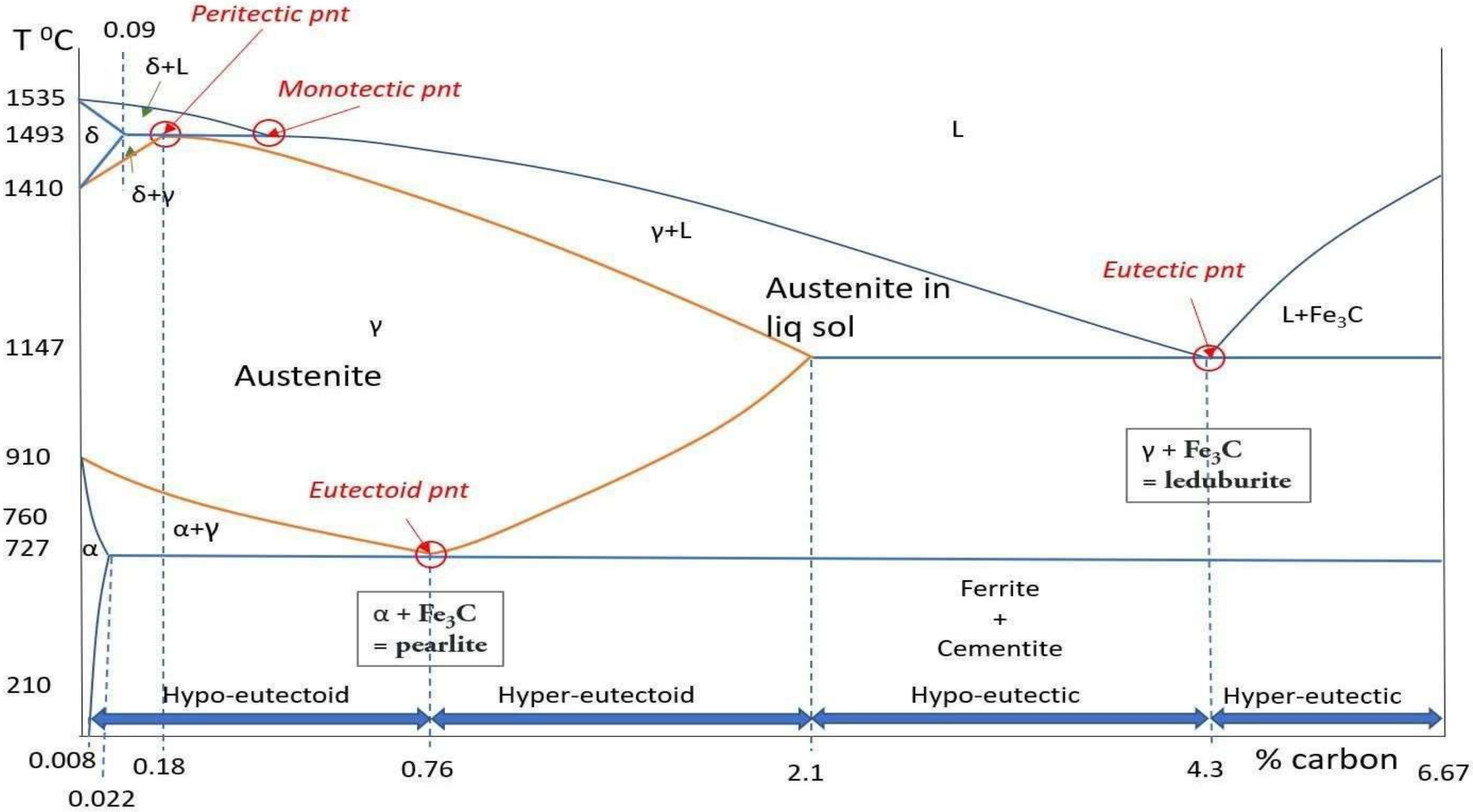
- $Fe-Fe_3C$ phase diagram is characterized by five individual phases,: **α**–ferrite (BCC) Fe-C solid solution, **γ**-austenite (FCC) Fe-C solid solution, **δ**-ferrite (BCC) Fe-C solid solution, Fe_3C (iron carbide) or cementite - an inter-metallic compound and liquid Fe-C solution and four invariant reactions:

- **peritectic reaction** at 1495 °C and 0.16%C, **δ**-ferrite + **L**↔ **γ**-iron (austenite)
- **monotectic reaction** 1495 °C and 0.51%C, **L** ↔ **L** + **γ**-iron (austenite)
- **eutectic reaction** at 1147 °C and 4.3 %C, **L** ↔ **γ**-iron + Fe_3C (cementite) [ledeburite]
- **eutectoid reaction** at 723 °C and 0.8%C, **γ**-iron ↔ **α**– ferrite + Fe3C (cementite) [pearlite]

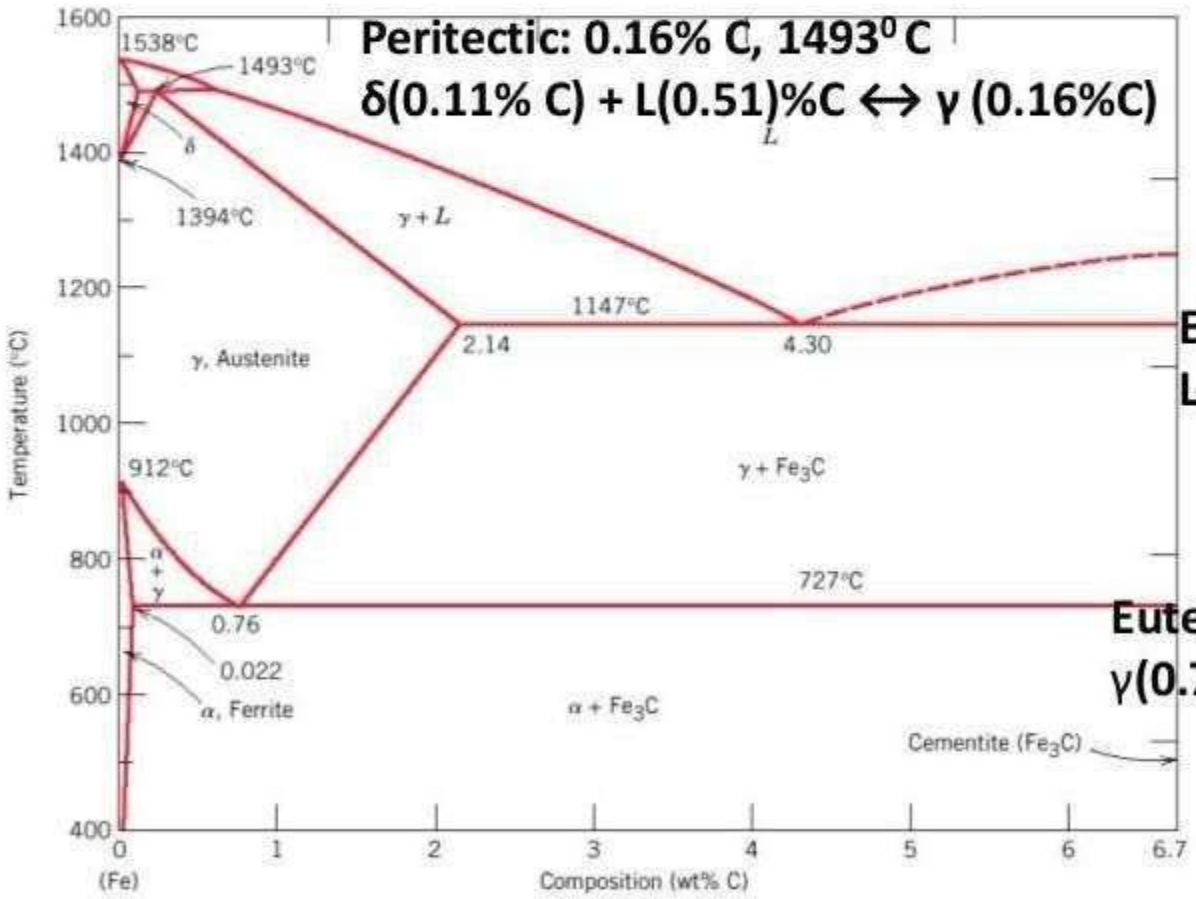
Contd...

w to draw iron carbon diagram | iron carbon diagram explained| iron carbon diagram




T °C
0.09
Peritectic pnt
δ+L
Monotectic pnt
1535
1493
δ
1410
δ+γ
L
γ+L
Eutectic pnt
Austenite in
liq sol
L+Fe3C
γ
1147
Austenite
910
γ + Fe3C
= leduburite
Eutectoid pnt
760
α+γ
727
α
Ferrite
+
Cementite
α + Fe3C
= pearlite
210
Hypo-eutectoid
Hyper-eutectoid
Hypo-eutectic
Hyper-eutectic
0.008
0.18
0.76
2.1
4.3
% carbon
6.67
0.022

Important Reactions in Fe–C System



Peritectic: 0.16% C, 1493^0 C

δ(0.11% C) + L(0.51)%C $\leftrightarrow$ γ (0.16%C)

Eutectic: 4.30 wt% C, 1147 °C

L (4.30% C) $\leftrightarrow$ γ (2.14% C) + Fe_3C

Eutectoid: 0.76 wt%C, 727 °C

γ(0.76% C) $\leftrightarrow$ α (0.022% C) + Fe_3C

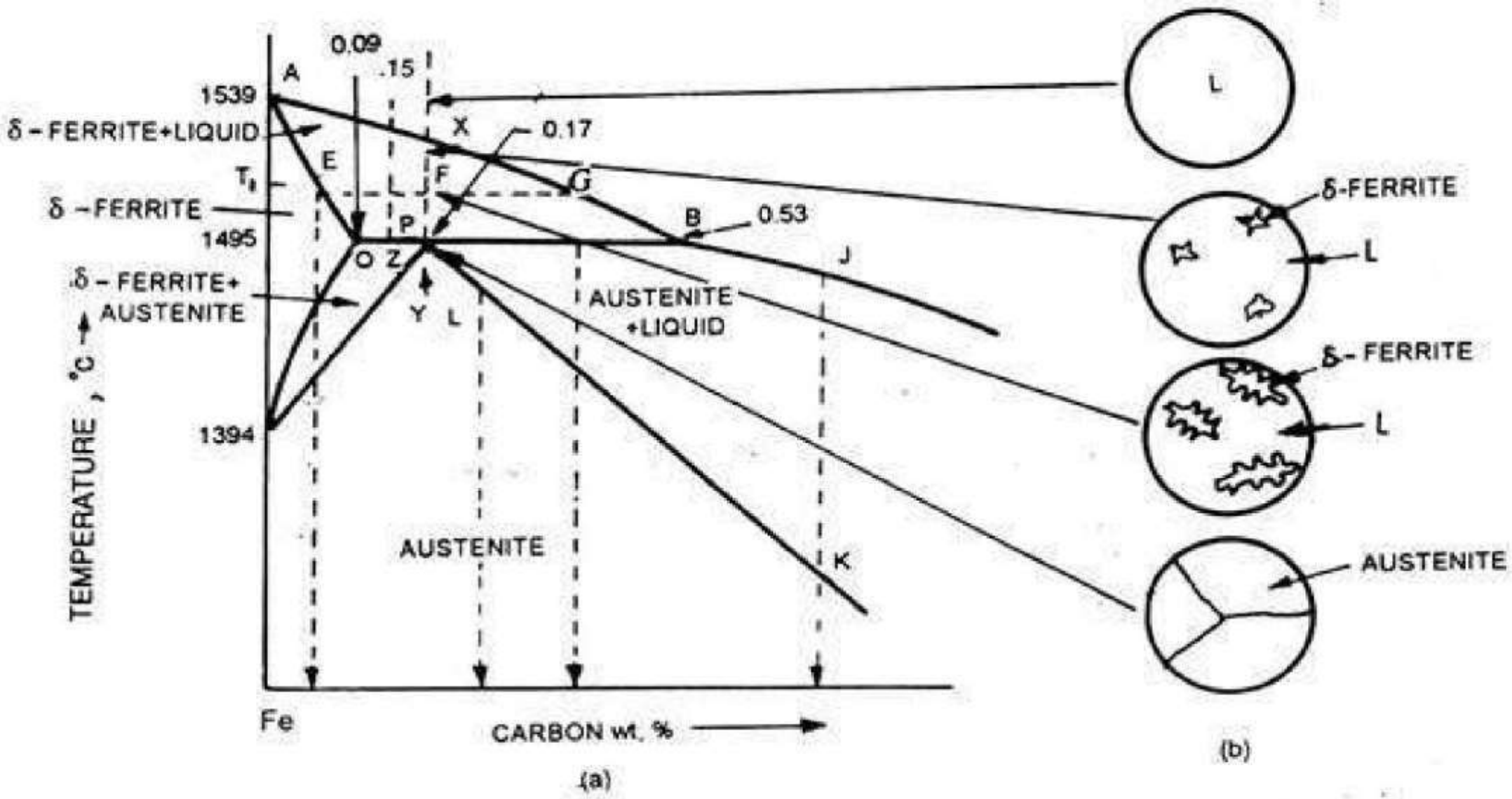


Fig. 1.23 Peritectic region of Fe-Fe_3C diagram

Reactions

Peritectic $L + \delta = \gamma$
at T=1493°C and 0.18wt%C

Eutectic $L = \gamma + Fe_3C$
at T=1147°C and 4.3wt%C

Eutectoid $\gamma = \alpha + Fe_3C$
at T=727°C and 0.77wt%C

Max. solubility of C
in ferrite=0.022%
in austenite=2.11%

Phases Present

L

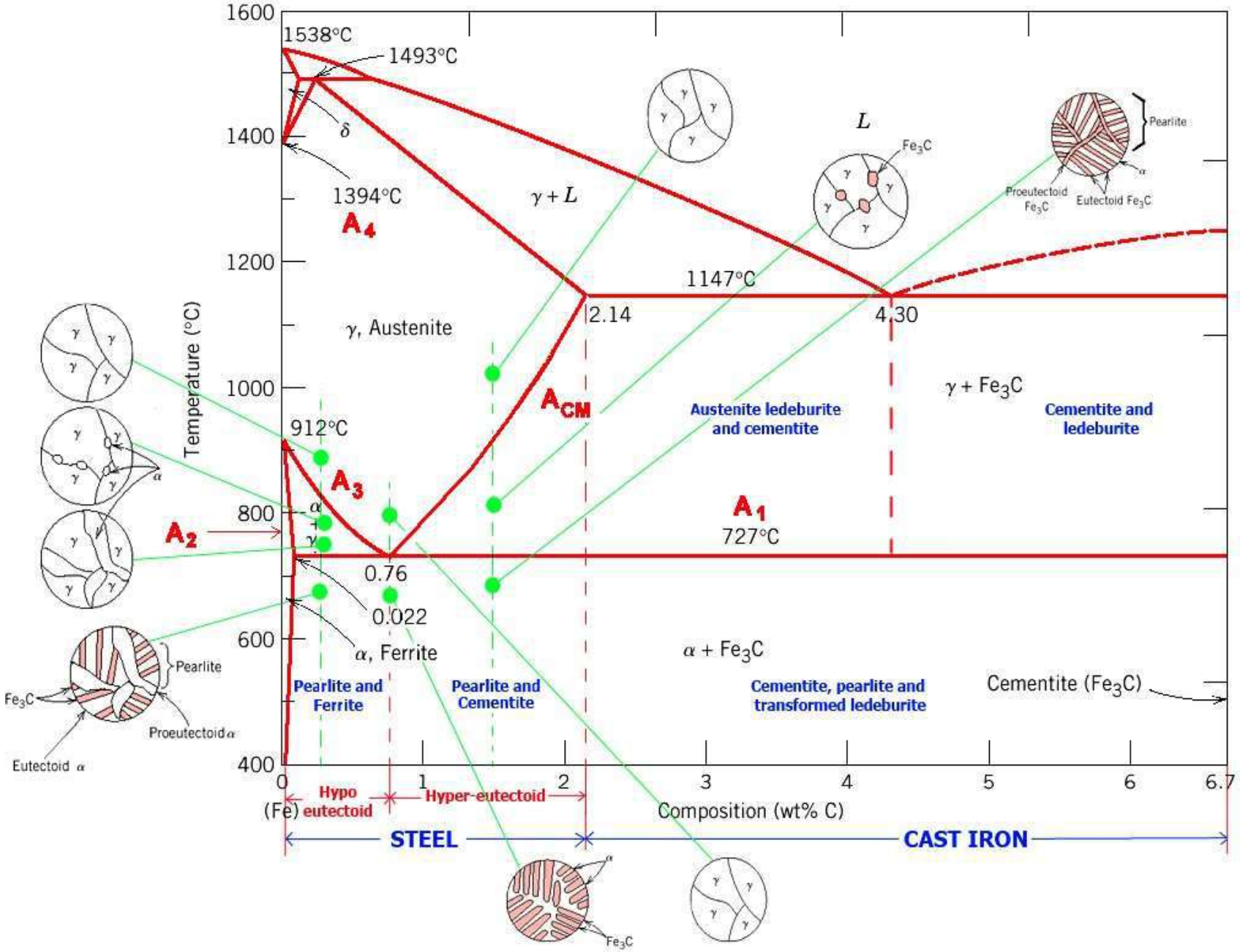
δ ferrite delta
Bcc structure
Paramagnetic

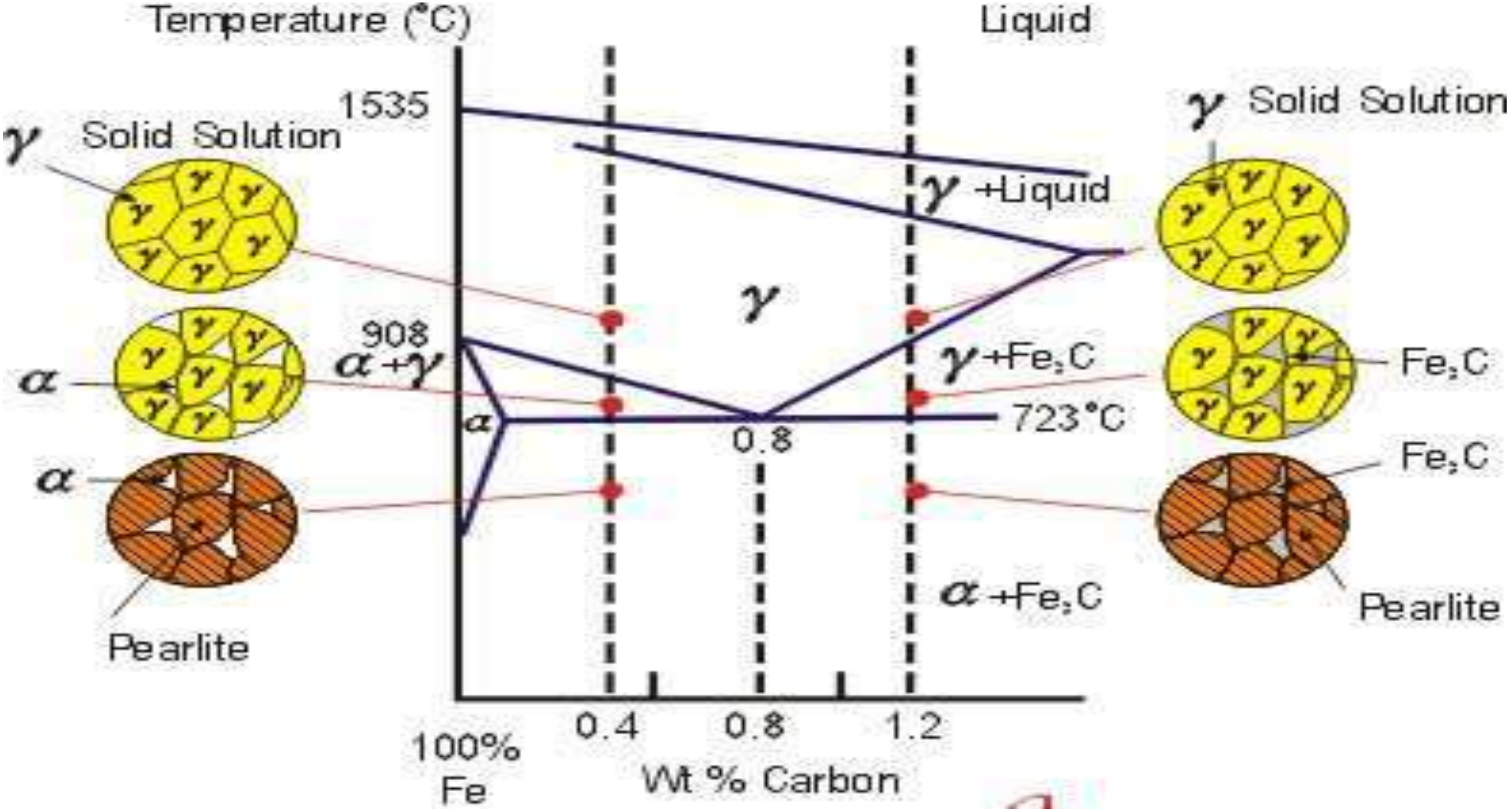
γ austenite
Fcc structure
Non-magnetic
ductile

α ferrite
Bcc structure
Ferromagnetic
Fairly ductile

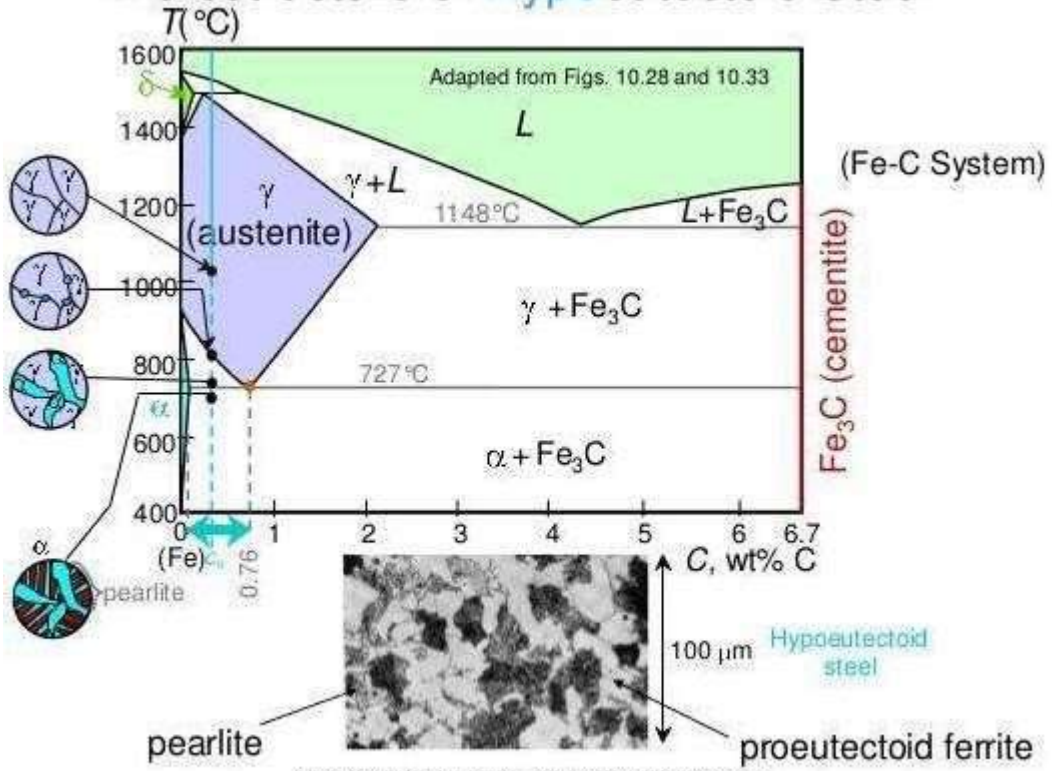
Fe_3C cementite
Orthorhombic
Hard, brittle

Microstructure of various phases



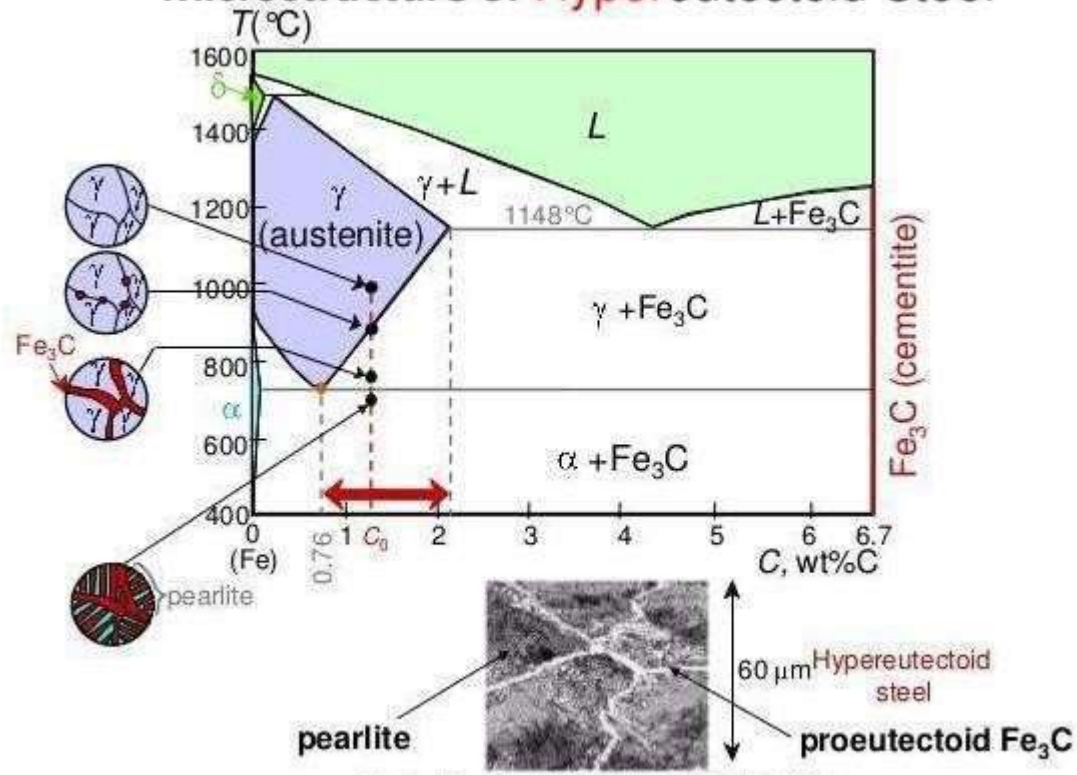

Temperature (°C)
Liquid
1535
γ Solid Solution
γ +Liquid
γ
908
α +γ
γ +Fe₃C
Fe₃C
723°C
0.8
α
Fe₃C
α +Fe₃C
Pearlite
Pearlite
0.4
0.8
1.2
100% Fe
Wt % Carbon

Microstructure of Hypoeutectoid Steel



Adapted from Fig. 10.34, *Callister & Rethwisch 3e.*

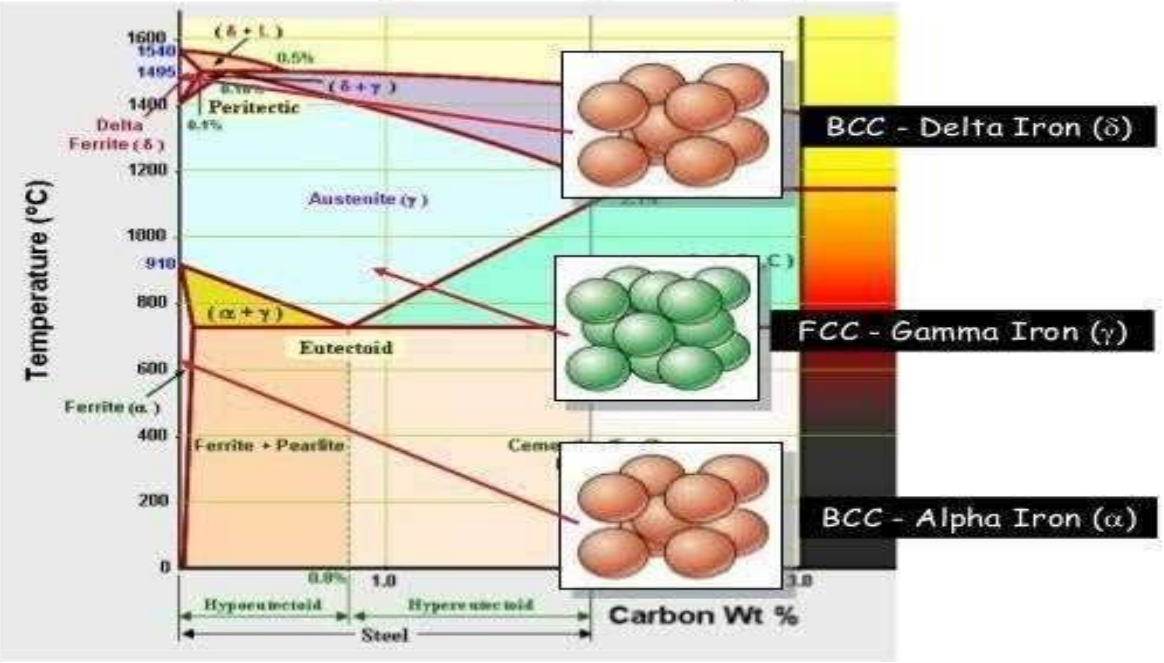
Microstructure of Hypereutectoid Steel



Adapted from Fig. 10.37, *Callister & Rethwisch 3e.*

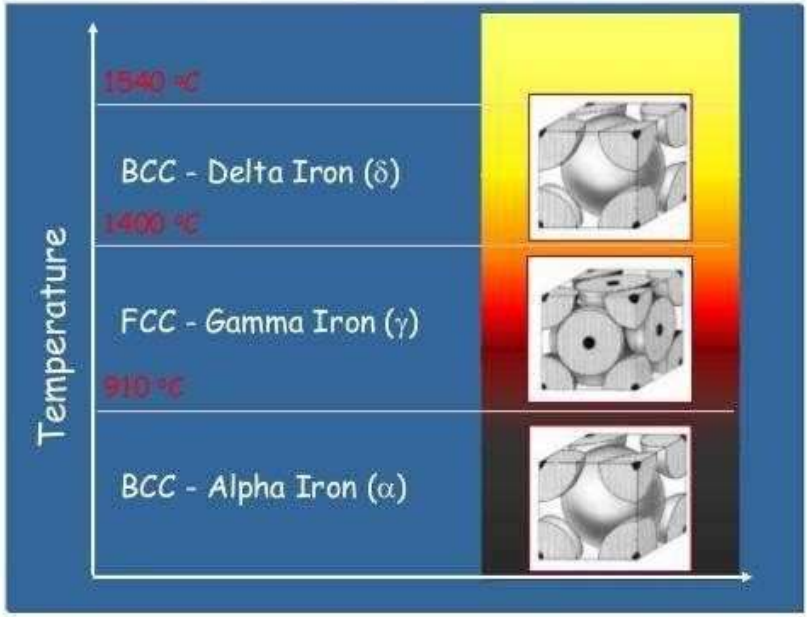
Basic Metallurgy

Atomic Packing in Iron (Allotropic)



Basic Metallurgy

Atomic Packing in Iron (Allotropic)



The Austenite to ferrite / cementite transformation in relation to Fe-C diagram

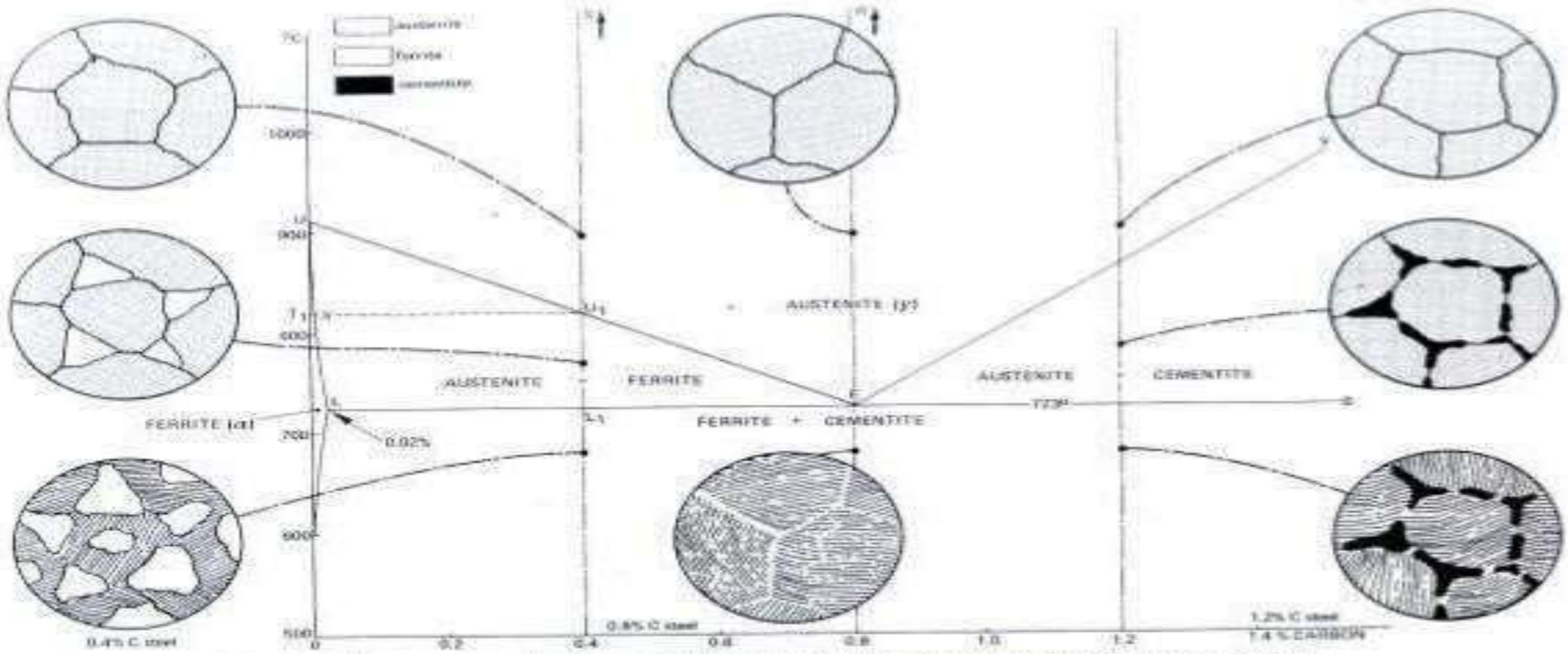


Fig. 9.3 The austenite → ferrite cementite transformation in relation to the iron-carbon diagram.

Alpha ferrite or α-ferrite:

- **Interstitial solid solution of carbon in iron of body centred cubic crystal structure (BCC) (α iron)(same as Fig. 2(a)).**
- **Maximum C solubility of 0.022% at 727°C.**
- **The stability of the phase ranges between low temperatures to 910°C, and solubility ranges 0.00005 wt % C at room**
- **Soft and ductile.**
- **Magnetic up to the Curie temperature of 768°C.**

Solid solution: one or more solute in the solvent, such as mixture, crystal structure remain unchanged by addition of solutes.

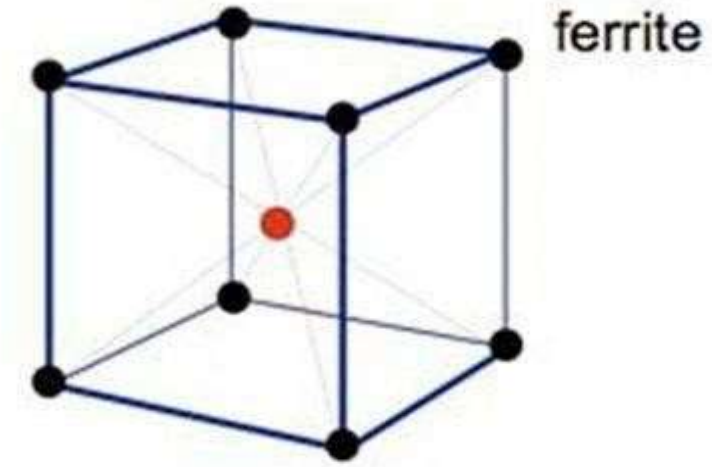
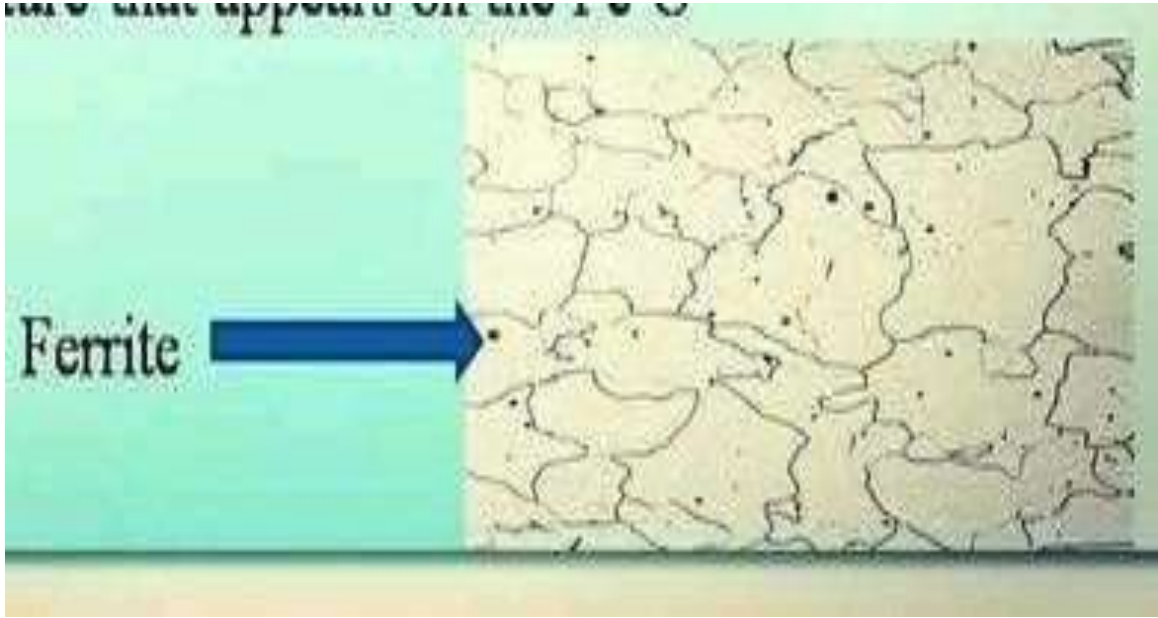


Fig.2(a): Crystal structure of ferrite



Austenite (γ)

M FACTS

- It is an interstitial solid solution of a small amount of carbon dissolved in γ iron.
- The maximum solubility is 2.1%C at 1147°C
- The crystal structure of Austenite (γ) is F.C.C.
- Hardness - 40 HRC and Toughness is high.

Cementite (Fe_3C)

M FACTS

- Cementite or iron carbide, chemical formula Fe3C, contains 6.67%C by weight.
- It is a metastable phase.
- Crystal structure is orthorhombic
- Typically hard and brittle interstitial compound.
- The hardest structure that appears on the Fe-C diagram.

Cementite network

Cementite

- This is also known as Iron Carbide (Fe_3C)
- It's a chemical compound because it contains a fixed percentage of carbon (6.67%)
- It has an orthorhombic crystal structure ($a \neq b \neq c$)

Ledeburite

- It is the eutectic lamellar mixture of austenite (light phase) and cementite (dark phase)
- It is unstable below 727°C and transforms into **α-ferrite and cementite.**

Pearlite

- Austenite containing 0.8% C forms pearlite upon slow cooling below 727°C
- Its lamellar structure of **α-ferrite and cementite.**
- It is very bright in appearance (like a pearl)
- It has a fingerprint like appearance