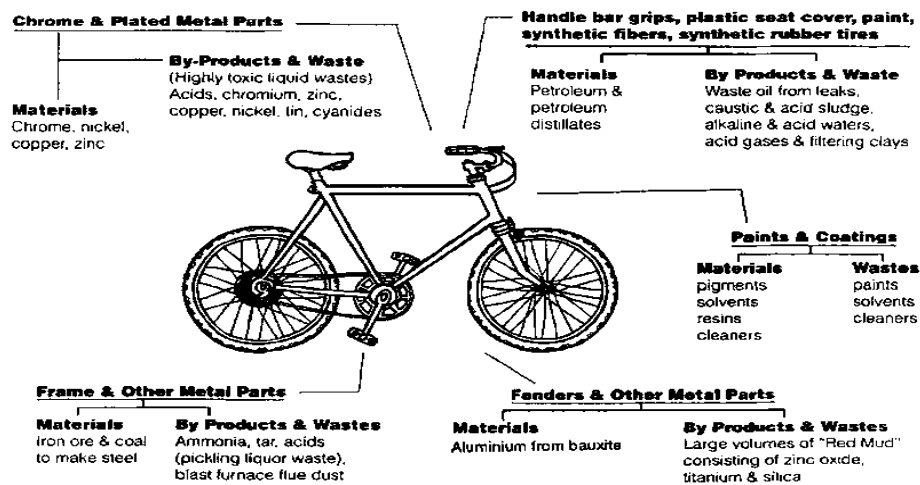# Module-I Material Science and Engineering

- Science is the intellectual and practical activity encompassing the systematic study of the structure and behaviour of the physical and natural world through observation and experiment.

- Engineering is the action of working artfully to bring something about.

Diversity of Materials

Classification: Metals are excellent conductors and ductile, such as steel and aluminum.
• Ceramics: High strength, brittle materials, such as glass and silicon carbide.
• Polymers: Lightweight and flexible materials, such as plastics and rubber.
• Composites: A combination of materials engineered for qualities, such as fiberglass.
• Semiconductors: Materials with intermediate conductivity, such as silicon and germanium.

Levels of Structure

- •Atomic structure includes many types of atoms as well as bonding.

- •The arrangement of atoms in space is the crystal structure.

- •Grains and phases - seen under a microscope are referred to as microstructure.

- •The overall material composition and imperfections that are visible to the human eye are referred to as the macrostructure.

Space lattice and Unit Cell

- Space Lattice is a three-dimensional collection of dots that represent the positions of atoms.
  Unit Cell -The smallest repeated unit in lattice, distinguished by the following elements:
  (Edge lengths) a, b, and c are the parameters of the lattice.
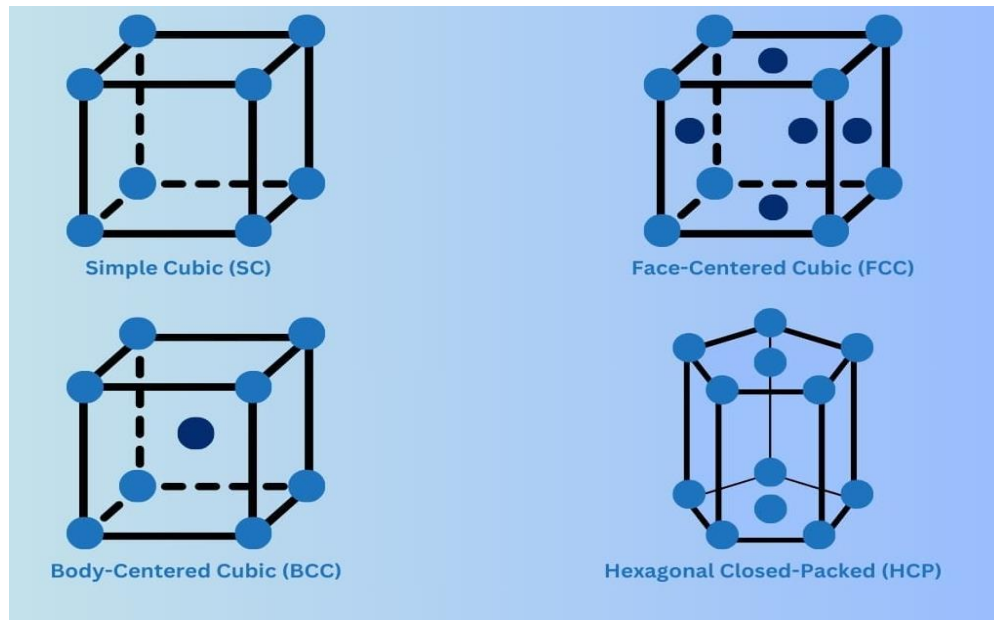 Angles: α, β, and γ (between three edges).

Metallic Crystal Structures

- At the corners of the simple cube (SC) are atoms.
- The number of coordination is six, and the efficiency of packing is fifty-two percent.
- Atoms are positioned at the corners and the center of the (body-centered cubic)- (BCC) structure.
- Packaging efficiency was 68%, and the coordination number was 8.
- Atoms will be positioned in the corners and face centers of the (face-centered cubic)- (FCC) type.
- 12 is the number of coordination, and 74% is the efficiency of packing.
- Atoms stacked in hexagonal layers are referred to as hexagonal close-packed (HCP) atoms.
- 12 is the number of coordination, and 74% is the efficiency of packing.

- While FCC metals have a high degree of ductility because they have several slip systems, HCP metals have a lower degree of ductility because they have fewer slip systems.

- Because of the more compact packing of atoms, FCC metals have a higher density than BCC and SC metals.

- At high temperatures, the crystal structure of certain metals, such as iron, undergoes a shift, resulting in the formation of FCC, while at ambient temperature, the structure of BCC is formed.

- Slip systems vary from structure to structure; for example, BCC has a moderate ductility, FCC has a high ductility because it has a large number of slip planes, and HCP has a limited ductility because it has restricted slip systems.

- BCC metals are normally tougher and stronger, but they are less ductile than FCC metals. On the other hand, FCC metals are softer and more ductile than HCP metals, whereas HCP metals are brittle yet strong in some applications.
- In comparison to BCC and HCP structures, FCC structures often have a higher thermal and electrical conductivity. This is because FCC structures have closer atomic packing together with superior electron mobility.
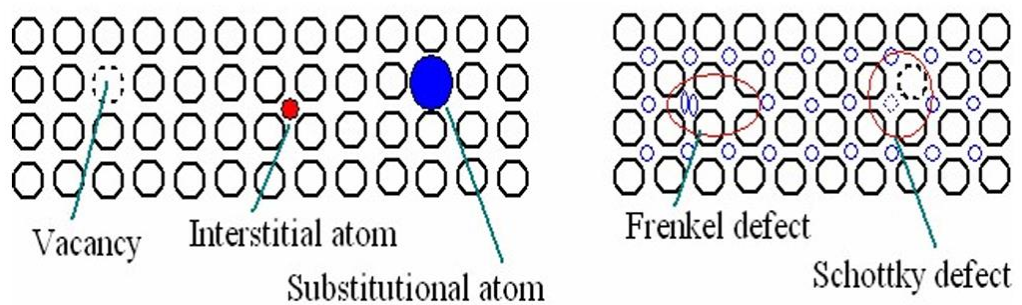
Metallic Crystal Structures

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
Tetrahedral Interstitial Sites	8	12

Simple Cubic (SC)

Face-Centered Cubic (FCC)

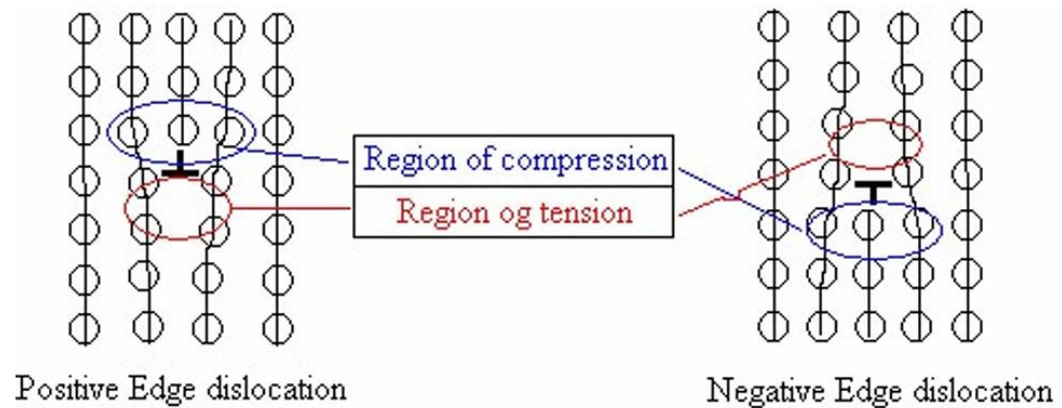Body-Centered Cubic (BCC)

Hexagonal Closed-Packed (HCP)

Crystal Imperfections

❖ Crystal defects are imperfections in the regular arrangement of elements within a crystal lattice that have a substantial impact on the properties of a material.

❖ Vacancies (absent atoms), interstitials (extra atoms in spaces), and substitutional defects (different atoms replacing host atoms) are all examples of point defects.
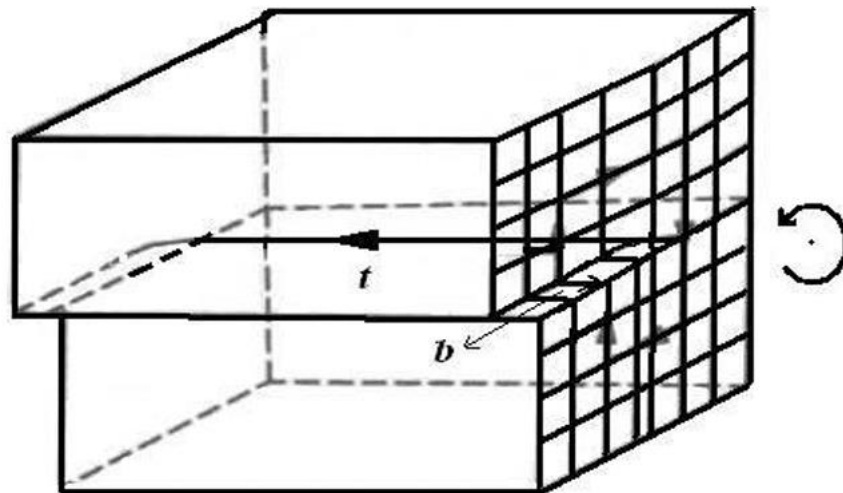

Vacancy   Interstitial atom

Substitutional atom

Frenkel defect

Schottky defect

Schematic depiction of various point defects

❖ Dislocations, or line defects, are irregularities that occur along a line within the lattice. They are frequently classified as screw dislocations and edge dislocations.
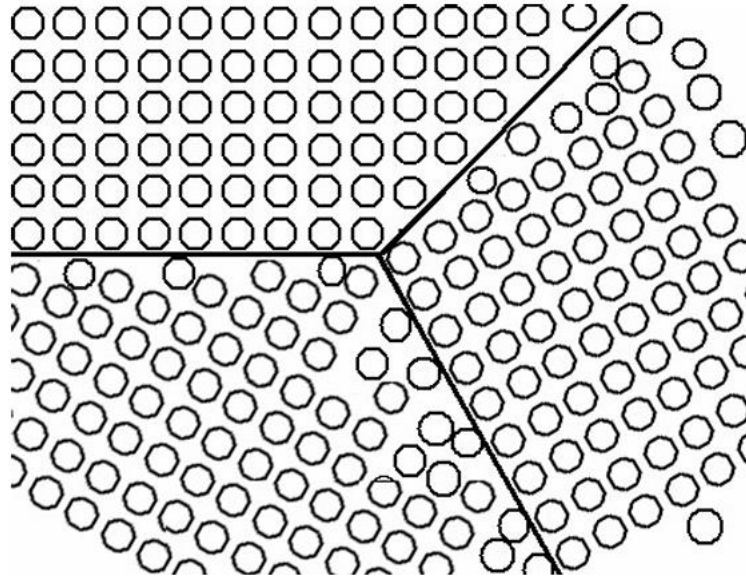

Positive Edge dislocation   Negative Edge dislocation

❖ Interstitial defects are the result of foreign atoms occupying the spaces between the regular atomic positions in the lattice.

❖ Volume defects, including voids, fractures, and inclusions, are three-dimensional imperfections that frequently compromise the material.
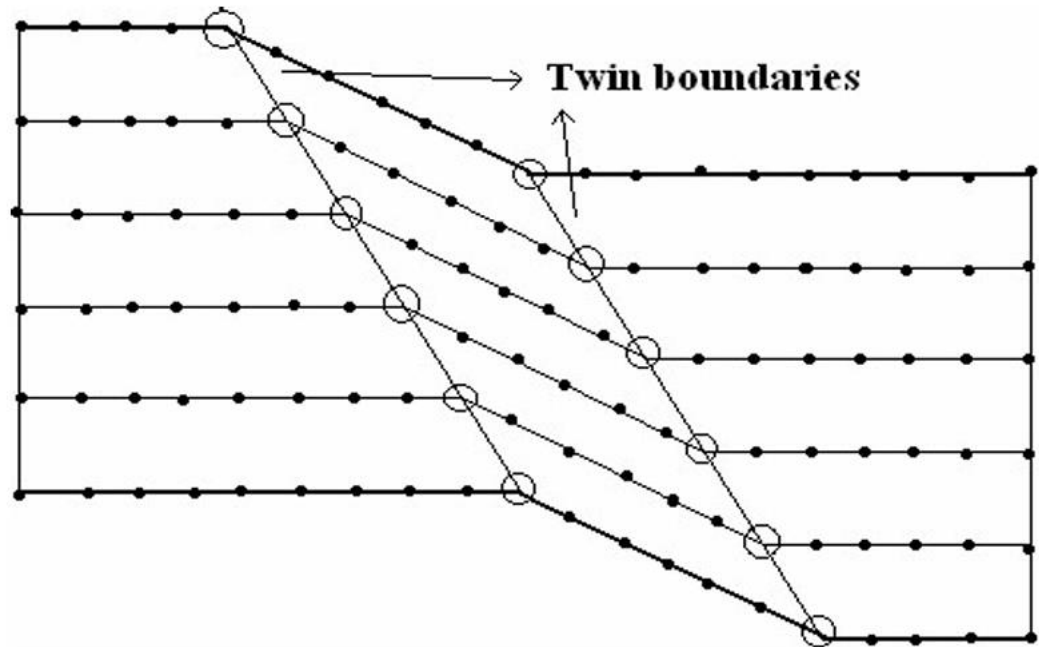

Negative screw dislocation.

❖ The presence of defects can improve ductility by facilitating dislocation movement; however, if they are present in excess, they may diminish strength.

Schematic presentation of grain boundaries

❖ The strength -of any material- is enhanced by the refining grain - boundaries, which serve as barriers to dislocation motion at the intersection of various crystal orientations.

❖ By allowing atoms to rearrange into a more stable structure, annealing processes can mitigate defects such as dislocations.

❖ Material properties, including conductivity, hardness, and corrosion resistance, are determined by the density and type of defects.
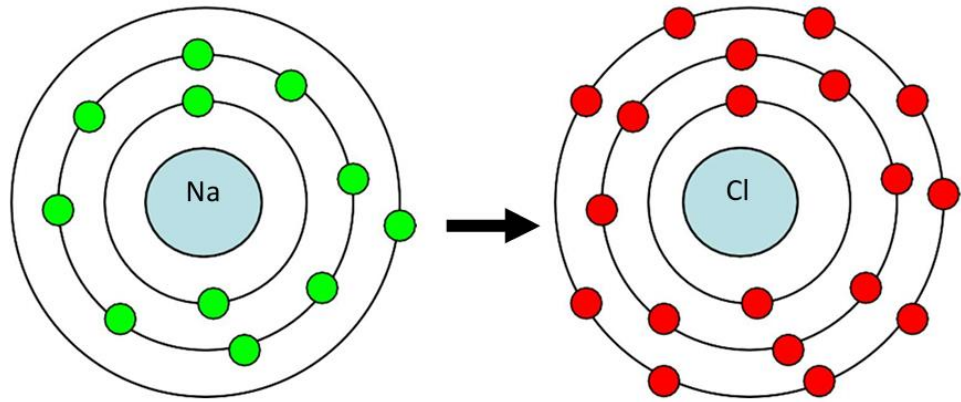
Twin boundaries

A pair of twin boundaries.

❖ The introduction of defects under controlled conditions, such as through alloying or work hardening, is employed to customize materials for specific applications.
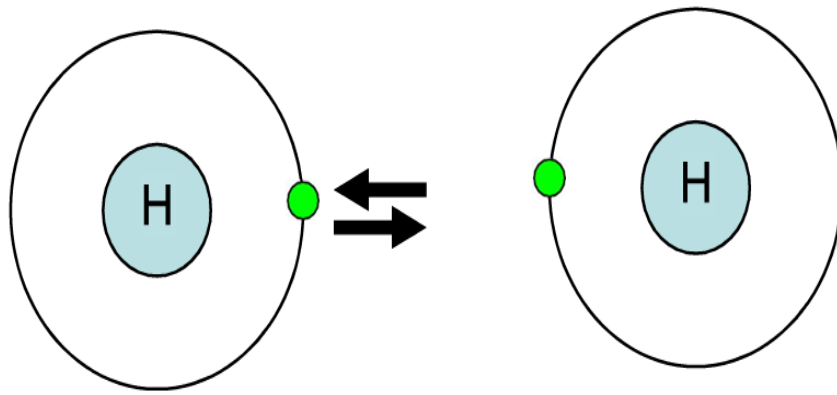
Bonding

❖ The interaction between atoms or molecules is governed by bonding in materials, which determines their mechanical, thermal, electrical, and optical properties.

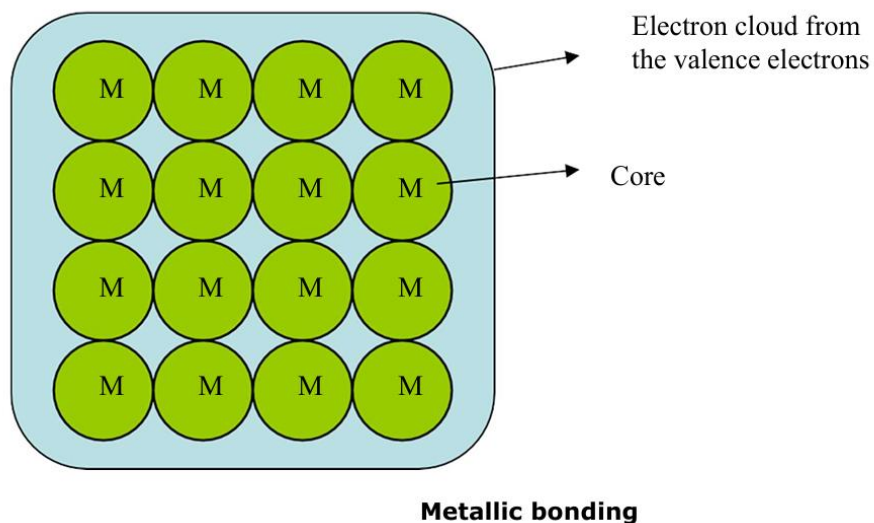❖ Primary bonds are distinguished by the sharing or transfer of

electrons and strong interatomic forces, and they include ionic, covalent, and metallic ones.

❖ Strong, brittle materials such as ceramics (e.g., NaCl) are the consequence of the formation of ionic bonds between atoms with significant differences in electronegativity.

❖ Covalent bonds, as seen in diamond or silicon, are formed by the sharing of electrons between elements with similar electronegativity, resulting in high strength and directional properties.

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❖ Metallic bonds are characterized by a "sea of delocalized electrons" that envelop positive metal ions, thereby enhancing their electrical conductivity, malleability, and ductility.

Metallic bonding

❖ Secondary bonds- including hydrogen- bonding and (van der Waals forces), are less robust than primary bonds; however, they are crucial to the properties of molecular materials and polymers.

❖ Van der Waals forces are generated by temporary dipoles in molecules, which result in mild attractions that affect properties such as melting and boiling points.

❖ Hydrogen bonds are a more potent form of secondary bonding that arise when an electronegative atom that is covalently bonded to a hydrogen atom interacts with another electronegative atom, as is the case in water.

❖ The hardness of a material is influenced by the type of bonding; ionic and covalent materials are generally harder, whereas metallic materials are more ductile but gentler.

❖ Thermal conductivity is also influenced by bonding. Metallic bonds exhibit high conductivity because of unrestricted electron movement, whereas covalent and ionic bonds restrict thermal flow.

Constitution of Alloys: Necessity of Alloying

❖ Alloying improves mechanical properties such as strength, hardness, and toughness, making metals suitable for demanding applications.
❖ It enhances corrosion resistance, as seen in stainless steel, where chromium prevents rust formation.
❖ Alloying alters thermal and electrical conductivity, tailoring materials for specific industrial uses like electrical wires or heat-resistant components.
❖ It allows for modification of physical properties like density, color, or magnetic behavior to meet specialized needs.
❖ The introduction of alloying elements refines grain structure, improving wear resistance and fatigue strength.
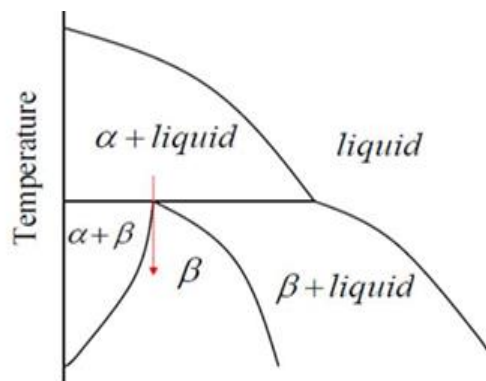
Constitution of Alloys: Necessity of Alloying

1. Gibbs's Phase Rule is denoted as $F=C-P+2$ and $F=C-P+2$, where F represents degrees of freedom, C represents the number of components, and P represents the number of phases.
2. It assists in determining the number of variables (such as temperature, pressure, or composition) that can be independently modified without affecting the number of phases.
3. The rule is essential for comprehending the equilibrium between phases in alloy systems and phase diagrams.
4. It clarifies the reason for the simpler phase diagrams of binary systems in comparison to ternary systems, which are attributed to the reduced number of components.
5. Alloy thermal treatment and the prediction of material behavior in multi-phase regions are practical applications.

Constitution of Alloys: Hume - Rothery's Rules for Solid Solubility

1. Hume Rothery rules govern the formation of solid solutions in alloy systems, emphasizing conditions for solubility.
2. Atomic size difference between elements should not exceed 15% to ensure minimal lattice distortion.
3. Components must have similar electronegativity to avoid compound formation instead of a solid solution.
4. Both elements should possess the same crystal structure for complete solubility (e.g., FCC-FCC or BCC-BCC).
5. Valency difference should be small, as higher valence solutes typically dissolve more readily in lower valence solvent metals.

Constitution of Alloys: The Lever principle

1. The approach is an instrument employed in phase diagrams to ascertain the proportion of coexisting phases at a specific temperature and composition.
2. It functions by establishing a horizontal tie-line that connects the phase boundaries at the specified temperature.
3. The fraction of one phase is directly proportional to the length of the tie-line opposite that phase, which is then divided by the total length of the tie-line.

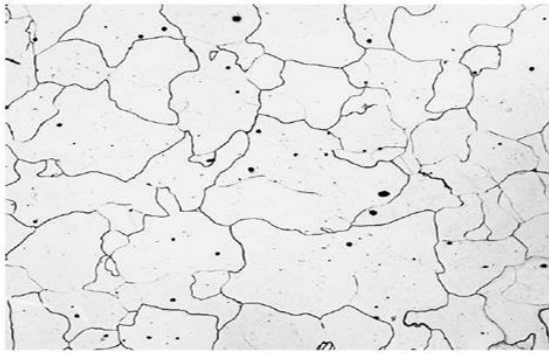3. The formula for the fraction of phase α is as follows:
5. $f\,\alpha$ = The length of the tie-line that is perpendicular to α
6. The total length of the tie-line
6. f α = The total length of the tie-line
7. The tie-line's length in the opposite direction of α

Alloy-1 / Liquid (L) / Liquidus / L+Y / Solidus / Temperature / M / α+Y / Y+B / Y₄ / E / Te / K / α+B / α+E.M. / B+E.M. / Composition / A / B / EM.: Eutectoid mixture / Primary α / Eutectoid (α+B) mixture / At point K

$$\underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}}$$

Solid₁ $\rightleftharpoons$ Solid₂ + Solid₃

Solid₁ / Solid₂ + Solid₃

An eutectoid diagram.

3. The lever rule is frequently employed to forecast microstructure proportions in binary alloy systems, including the Aluminum-Copper and Iron-Carbon systems.

4. An alloy system undergoes a eutectic reaction at a specific temperature and composition, during which a liquid phase undergoes a direct transformation into two solid phases simultaneously.

$$L \rightarrow \alpha + \beta$$

5. This reaction takes place at the eutectic point in a phase diagram, which is defined as the lowest temperature at which the alloy is entirely liquid.

A peritectoid diagram.

Solid₁ + Solid₂ $\underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}}$ New Solid₃

Solid₁ + Solid₂ / New Solid₃

5. Eutectic alloys, including lead-tin (Pb-Sn) solder, are distinguished by their exceptional castability and acute melting point.
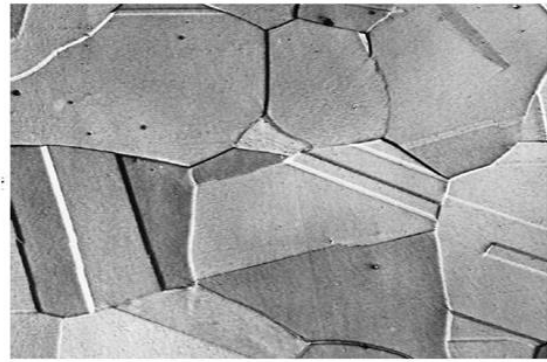
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6. A eutectoid reaction is characterized by the simultaneous transformation of a solid phase into two other solid phases: $\gamma \rightarrow \alpha + \beta$ γ→α+β

7. In the Iron-Carbon system, the eutectoid reaction takes place at 727°C and 0.8% carbon. Here, austenite (γ γ) undergoes a transformation into ferrite (α α) and cementite (Fe_3C Fe 3C), resulting in the formation of pearlite.
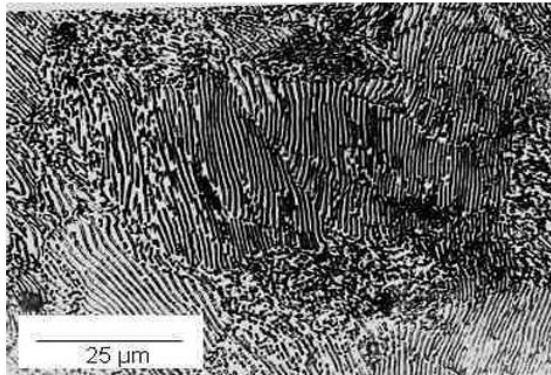
Iron-Iron Carbide (Fe-Fe₃C) diagram

- The Iron-Iron Carbide (Fe-Fe₃C) diagram illustrates the equilibrium between iron and carbon up to 6.67% carbon, corresponding to the composition of cementite (Fe₃C).
- The diagram includes essential phases: ferrite (α), austenite (γ), cementite (Fe₃C), and liquid iron (L), as well as the mixes pearlite, bainite, and martensite (resulting from rapid cooling).
- Ferrite (α) is a body-centered cubic (BCC) phase characterized by minimal carbon solubility (<0.02%), which imparts ductility but results in low strength.
- Austenite (γ) is a face-centered cubic (FCC) phase characterized by enhanced carbon solubility (up to 2.1%), which improves strength and ductility at increasing temperatures.
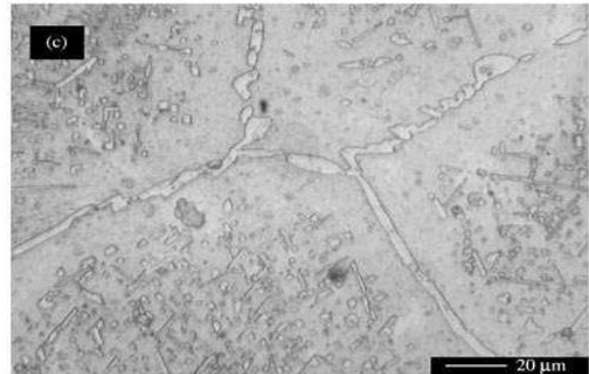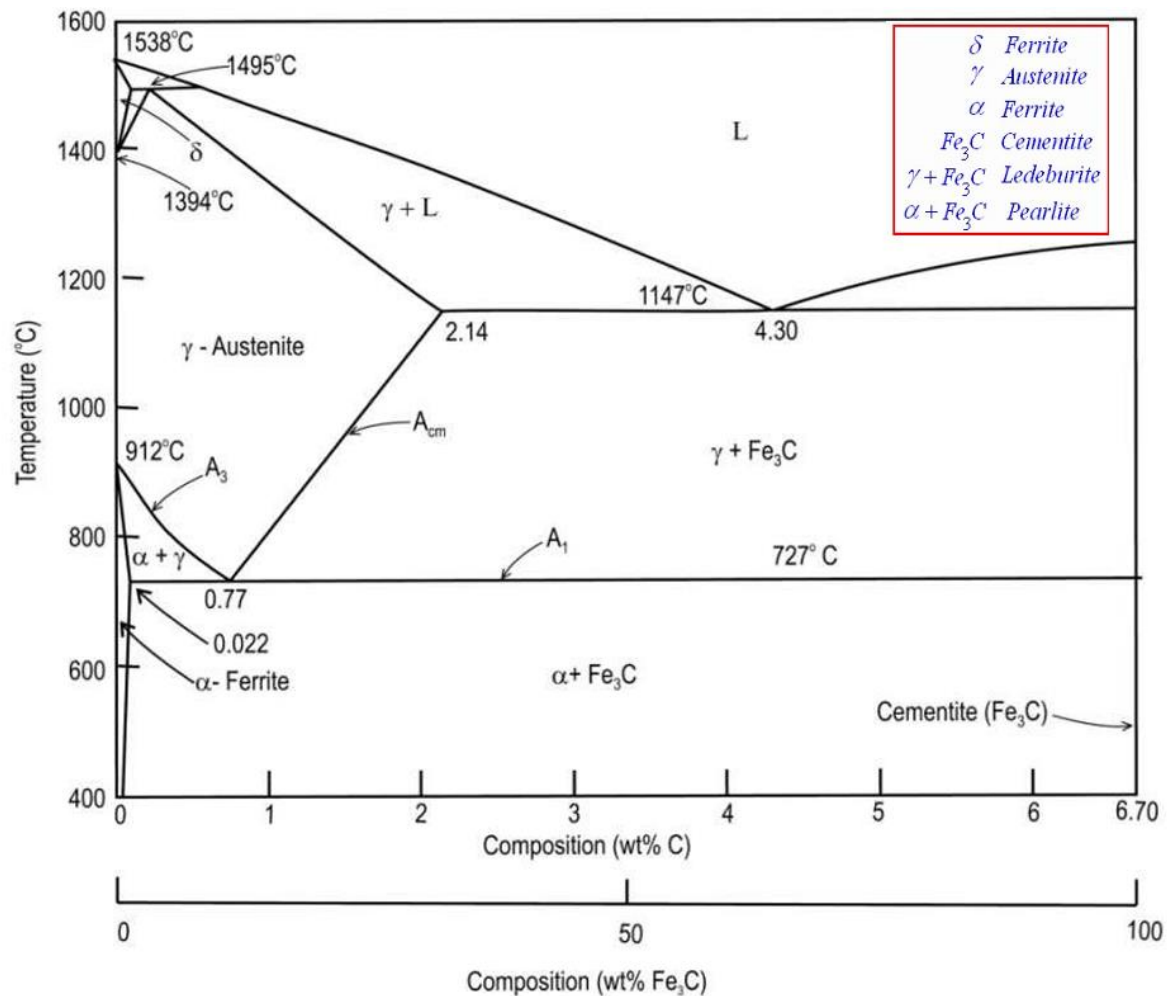
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a–ferrite
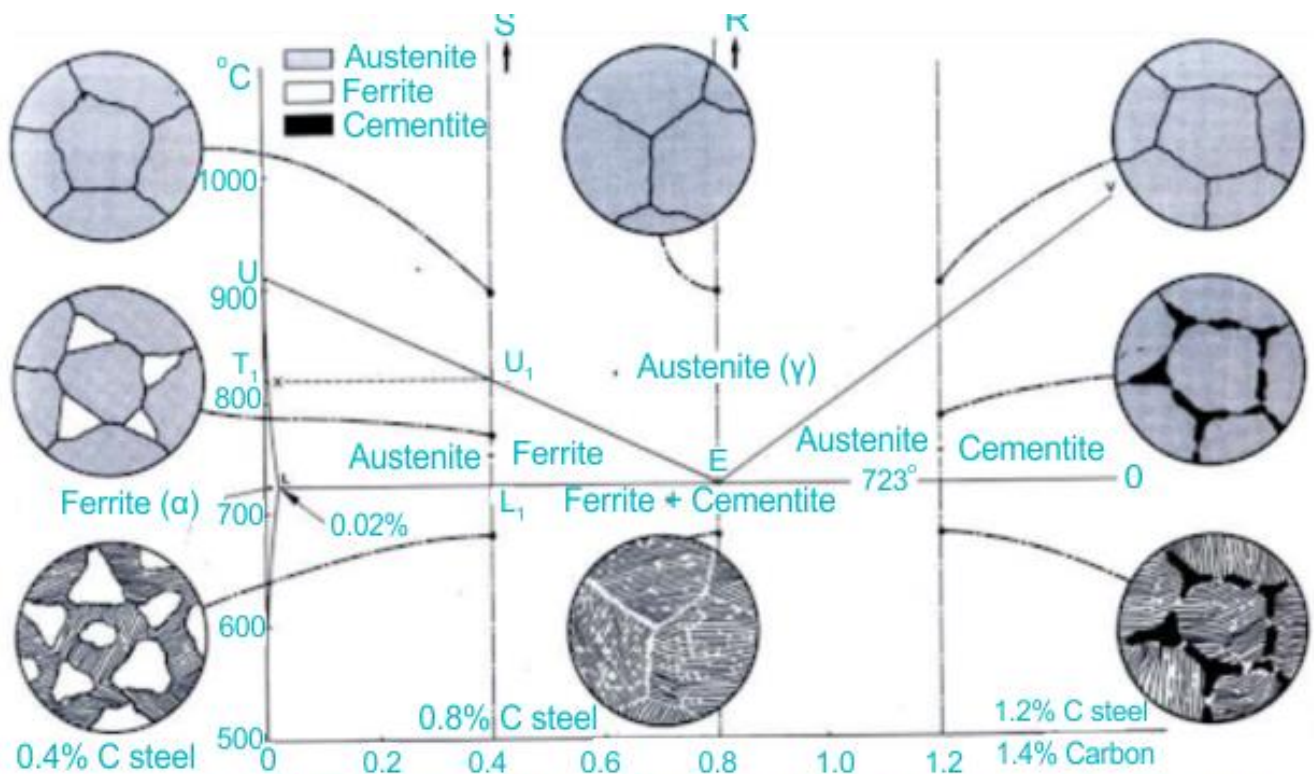
Austenite

Pearlite

Cementite

- Cementite (Fe_3C) is a rigid and brittle intermetallic compound that enhances hardness while diminishing ductility in steel.
- The eutectoid point is located at 0.8% carbon and 727°C, where austenite (γ) converts into pearlite, a lamellar configuration of ferrite (α) and cementite (Fe_3C).

- The eutectic point at 4.3% carbon and 1147°C signifies the simultaneous transformation of liquid into austenite and cementite, resulting in the production of ledeburite.
- Hypoeutectoid steels (carbon < 0.8%) comprise a combination of proeutectoid ferrite and pearlite, optimizing ductility and strength.
- Hypereutectoid steels (carbon > 0.8%) comprise proeutectoid cementite and pearlite, providing elevated hardness and wear resistance, albeit with reduced ductility.
- The Fe-Fe₃C diagram informs heat treatment procedures such as annealing, normalizing, and quenching to alter microstructures for certain mechanical properties in steels.

The Austenite → Ferrite/Cementite transformation in relation to the iron-carbon diagram