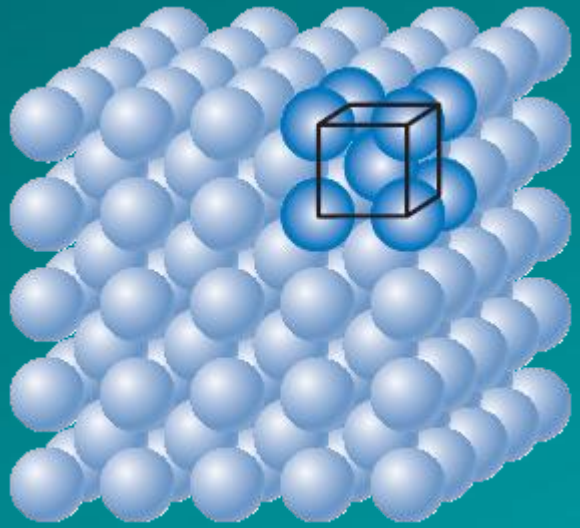
Materials Science and Engineering

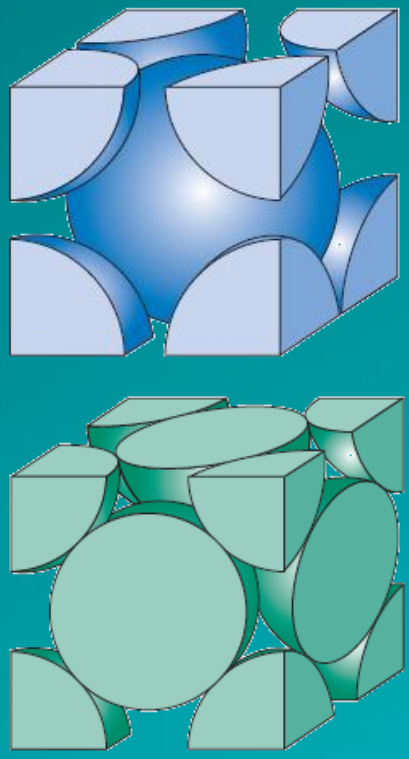
Atomic structure, Crystal lattice

Structure of crystalline solids

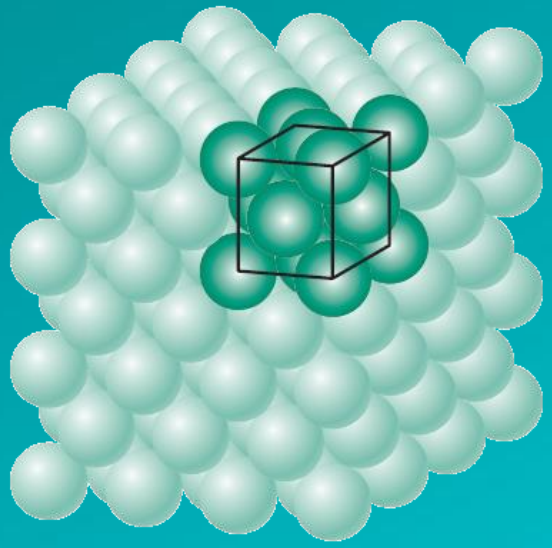
Lattice points: atoms, molecules, group of atoms. In ice the centre of the molecule is the lattice point.
Crystal: regular 3D pattern of atoms, molecules, group of atoms.
When describing crystalline structures, atoms (or ions) are thought of as being solid spheres having well-defined diameters. This is termed the atomic hard sphere model in which spheres representing nearest-neighbor atoms touch one another.



Body-centered cubic

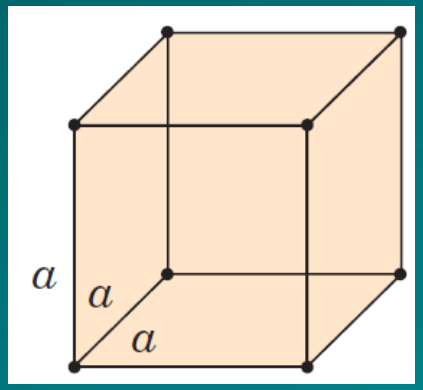


Face-centered cubic

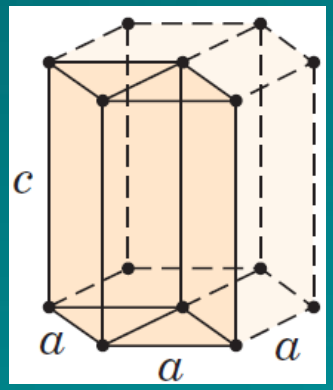


Structure of crystalline solids

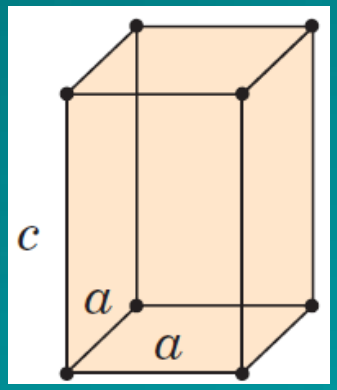
Our technical materials can form 7 types of primitive cells. All of the crystals, whether natural or synthetic, belongs to one of them.



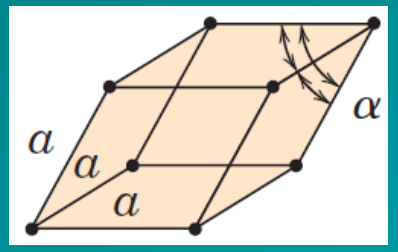
Cubic
a=b=c; α=β=γ=90°



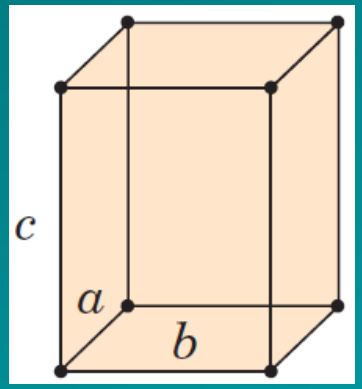
Hexagonal
a=b≠c; α=β=120°, γ=90°



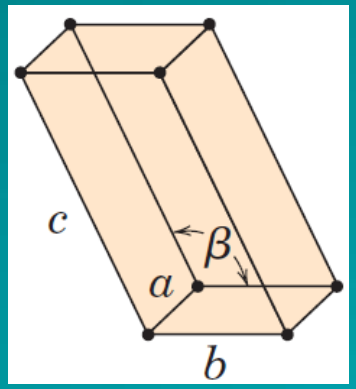
Tetragonal
a=b≠c; α=β=γ=90°



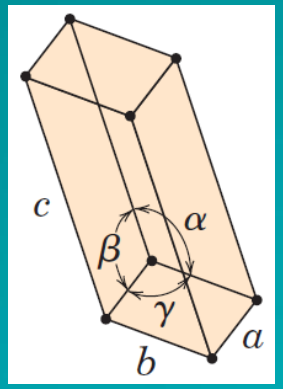
Rhombohedral
a=b=c; α=β=γ≠90°



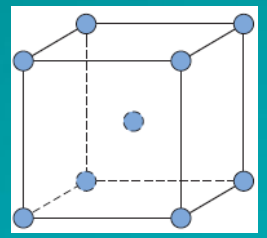
Orthorombic
a≠b≠c; α=β=γ=90°



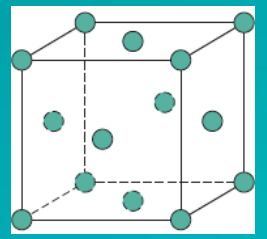
Monoclinic
a≠b≠c; α=γ=90°≠β



Triclinic
a≠b≠c; α≠β≠γ

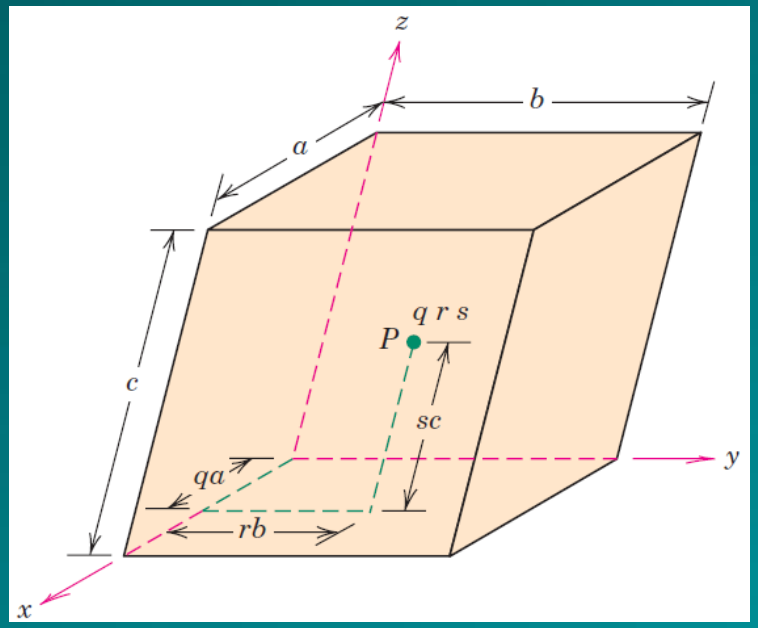


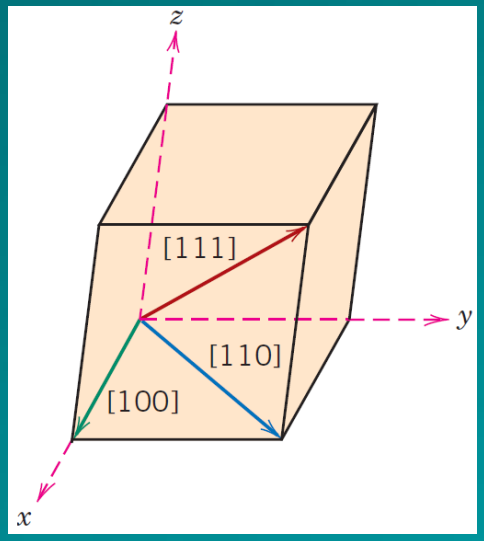
Body-centered cubic

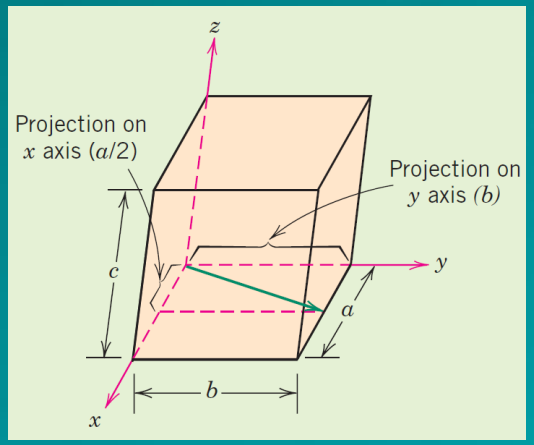


Face-centered cubic

Crystallographic directions and planes



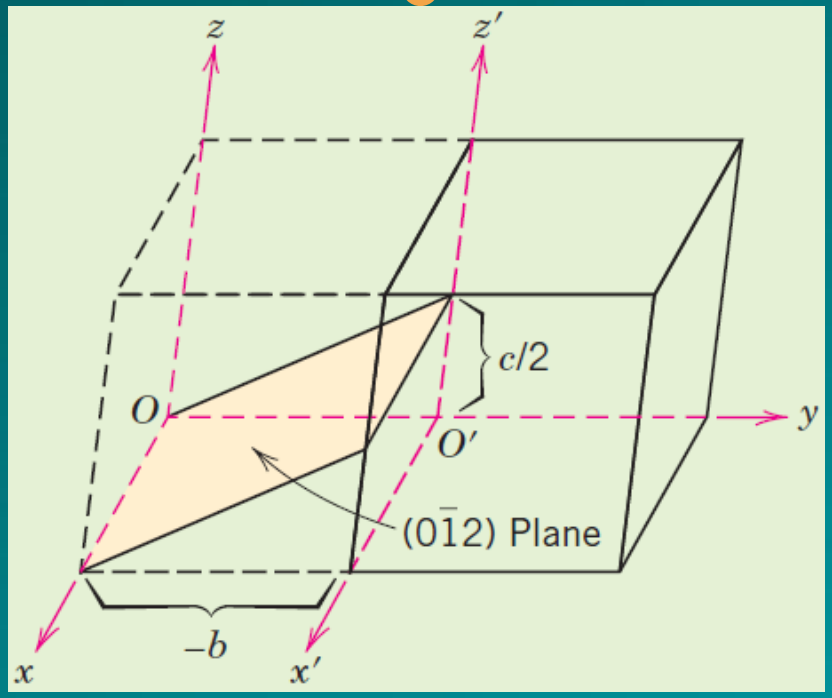


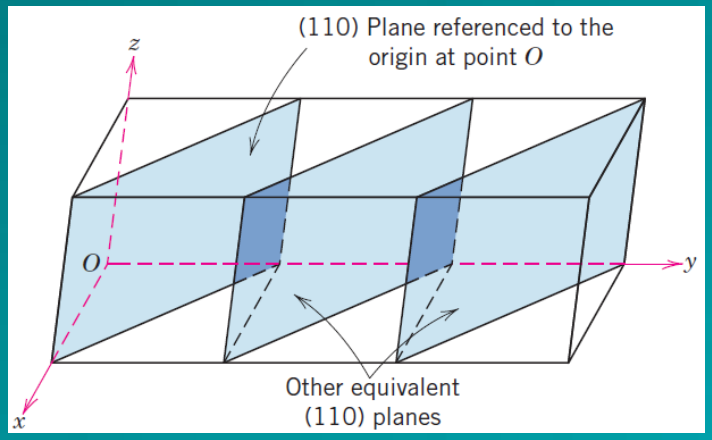


For some crystal structures, several nonparallel directions with different indices are actually equivalent; this means that the spacing of atoms along each direction is the same. For example, in cubic crystals, all the directions represented by the following indices are equivalent: [100], [-100], [010], [0-10], [001], and [00-1]. As a convenience, equivalent directions are grouped together into a family, which are enclosed in angle brackets, thus: <100>.

Miller indices.

Crystallographic directions and planes

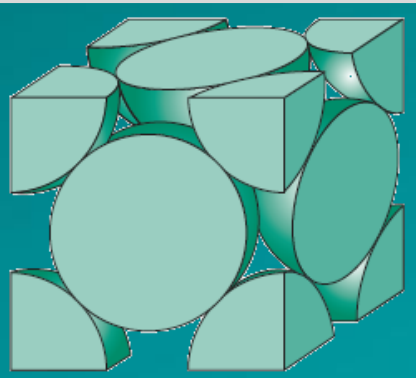




Since the plane passes through the selected origin O, a new origin must be chosen at the corner of an adjacent unit cell, taken as O'. This plane is parallel to the x axis, and the intercept may be taken as ∞a. The y and z axes intersections, referenced to the new origin O', are -b and, c/2 respectively. Thus, in terms of the lattice parameters a, b, and c, these intersections are ∞, -1 and ½. The reciprocals of these numbers are 0, -1, and 2; and since all are integers, no further reduction is necessary. Finally, enclosure in parentheses yields (0-12).

Also, in the cubic system only, planes having the same indices, irrespective of order and sign, are equivalent. For xample, both (1-23) and (3-12) belong to the {123} family.

Features of crystal structures

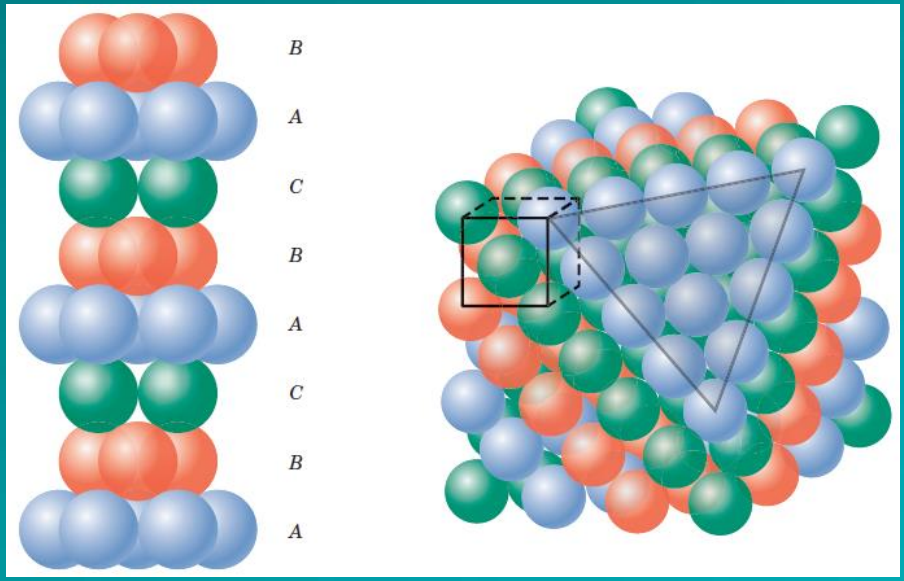


Coordination number: number of closest neighbours. FCC: 12

Atomic packaging factor: $atoms_{vol}/cell_{vol}$

Largest free space in the cell: The diameter of the biggest atom which can be put into the interstitial positions of the lattice without disturbing it. FCC: D=0,82r; and 0,45r.

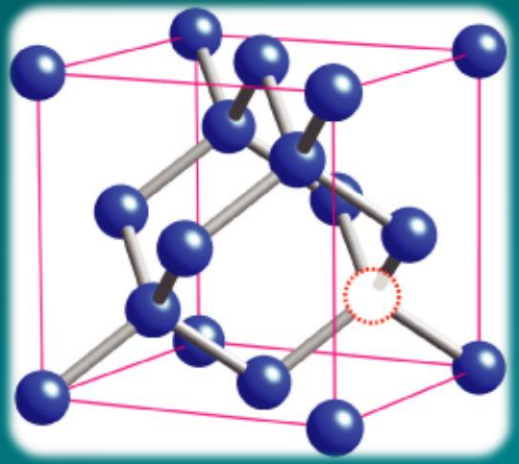
Closest packed direction: the direction where the linear density is the highest.
Closest packed planes: the planes where the planar density is the highest.

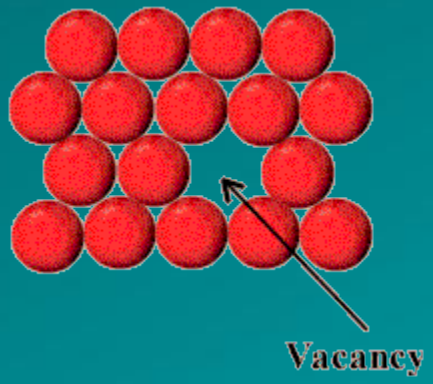


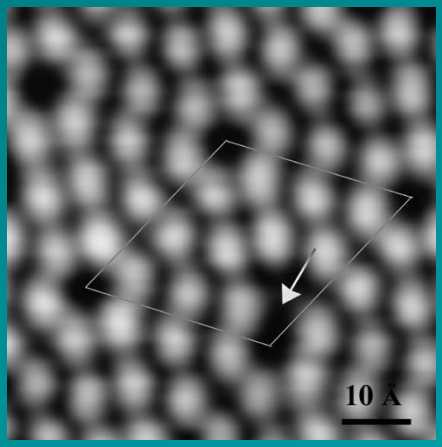
Materials Science and Engineering

Crystal defects

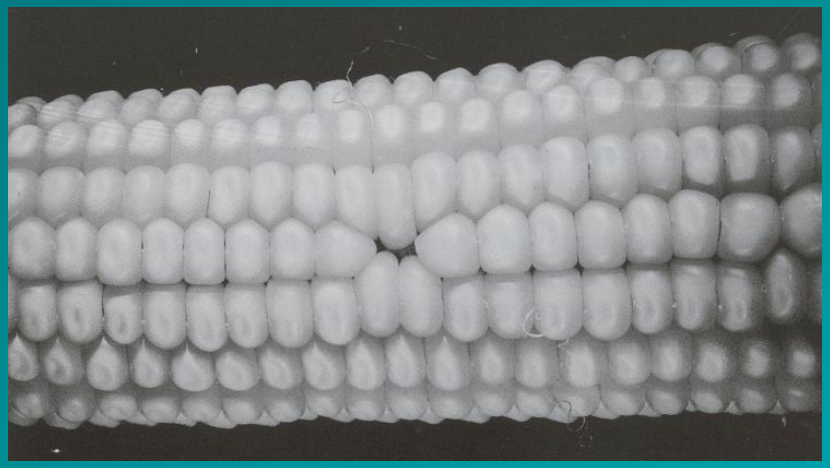
Point defects (oD)







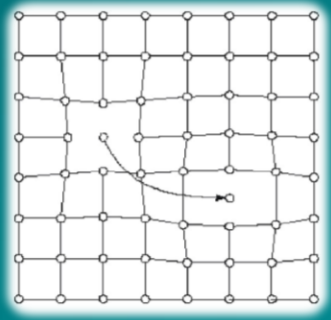
Vacancy: A defect wherein an atom is missing from one of the lattice sites is known as a 'vacancy' defect.

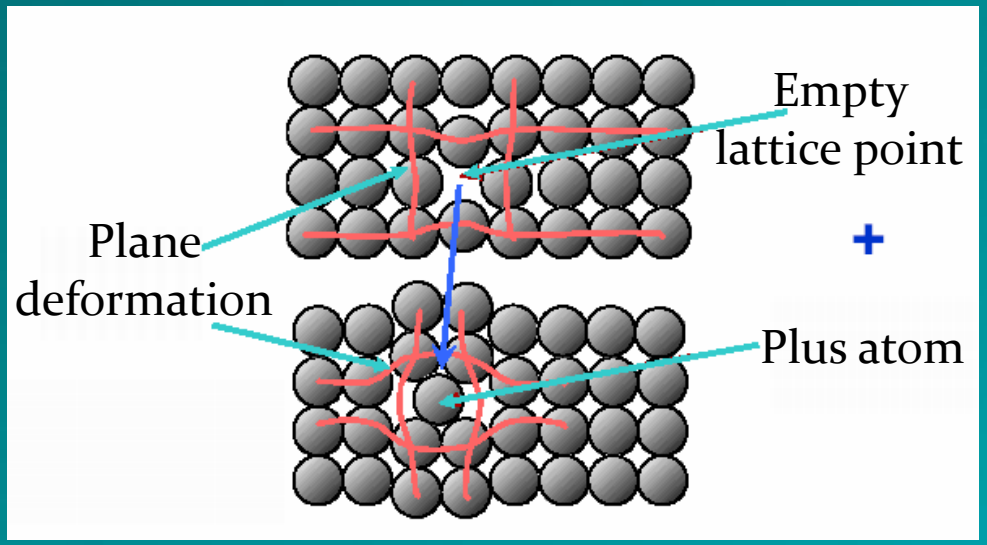


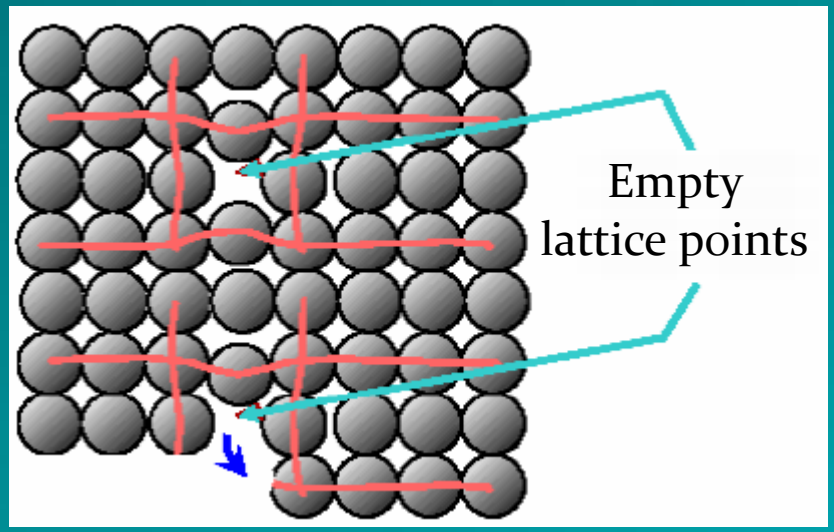
Point defects (oD)

Frenkel mechanism: An atom jumps out from its original position to a new place which is not a lattice point.

Need energy. Mostly in case of irradiation.

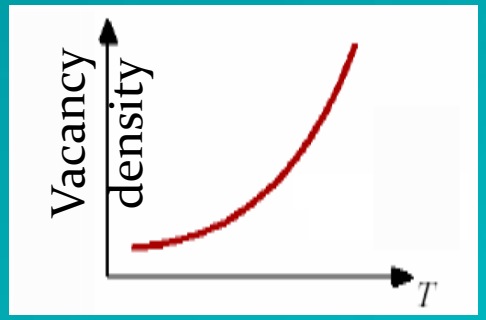






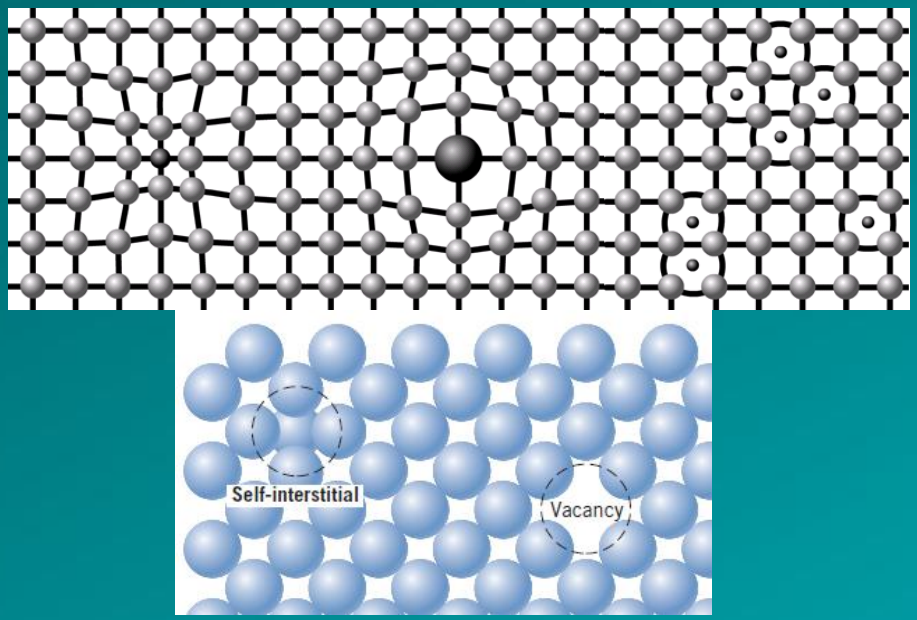
Wagner-Schottky mechanism: An empty lattice point „comes" from the surface into the metal (diffusion)

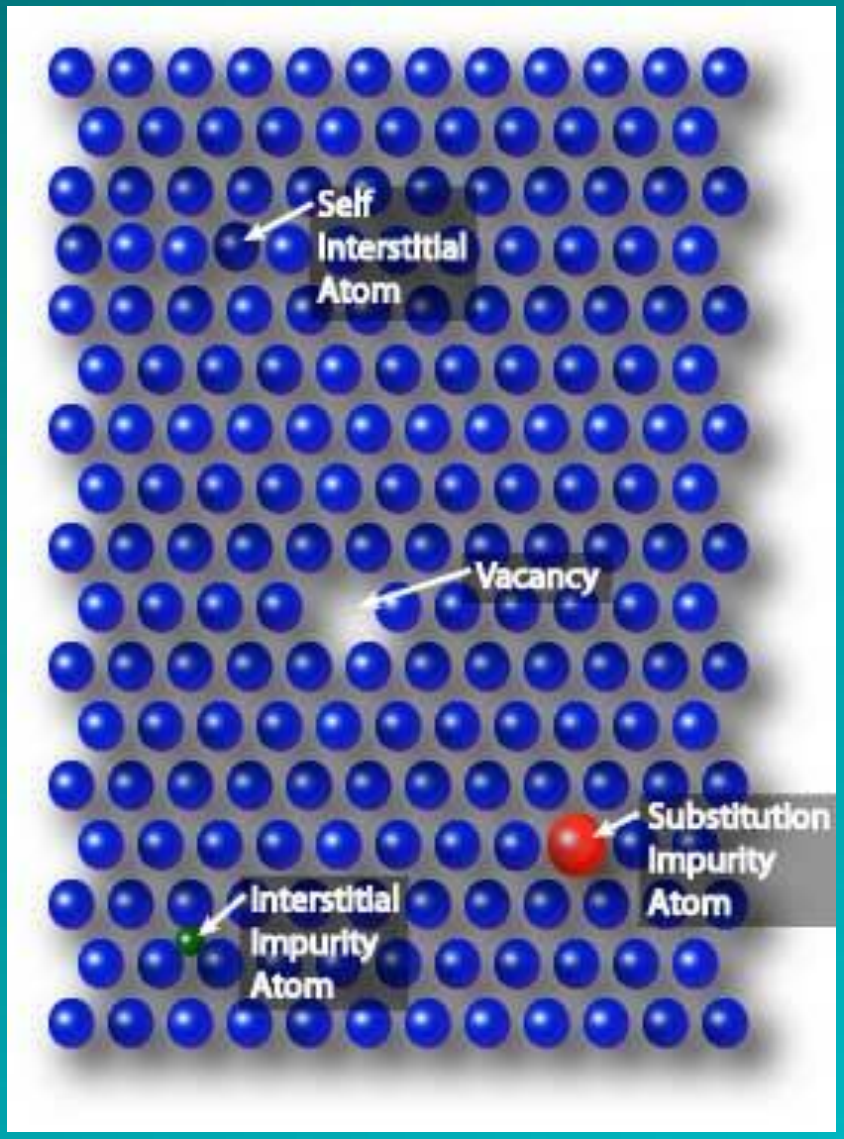
The heat gives energy for these processes.



Point defects (oD)

- Substitutional atoms
- Interstitial atoms
  - Self atoms
  - Impurity atoms

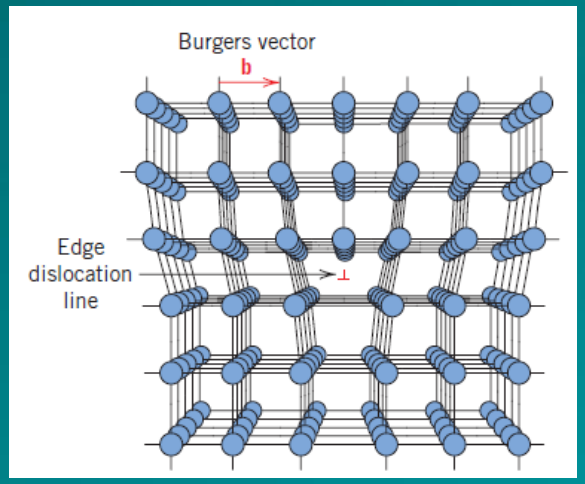


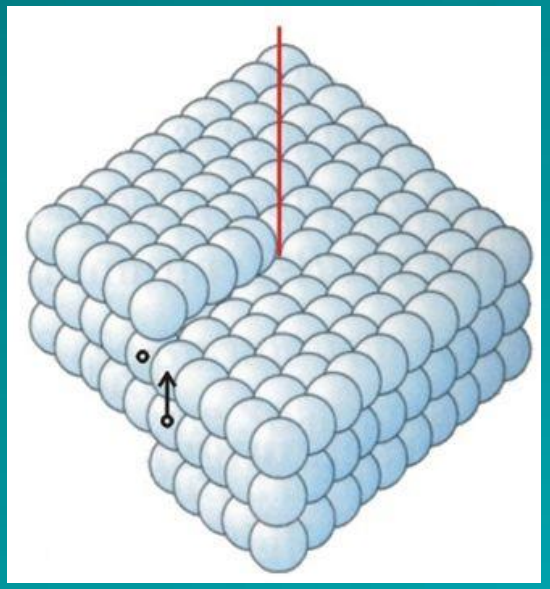


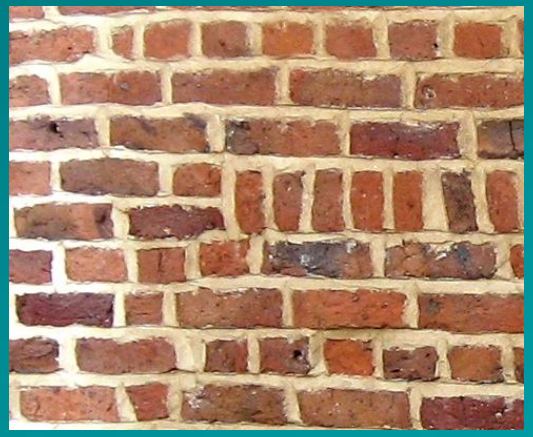
Theself interstitial and impurity atoms are deforming the lattice in both case. It is cause strengthening and decreasing in ductility.

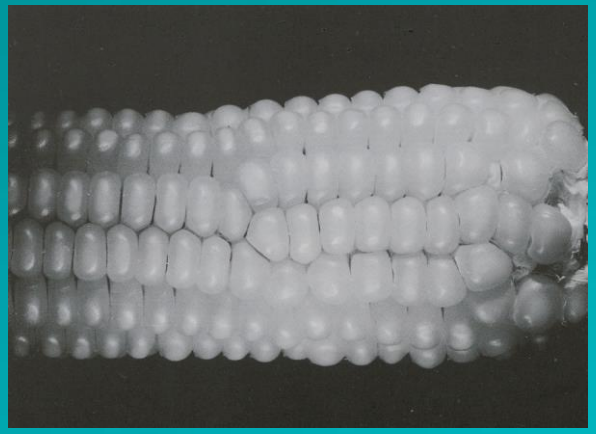
Linear defects (1D)

Edge dislocation: A dislocation is a linear or one-dimensional defect around which some of the atoms are misaligned. This is termed an edge dislocation; it is a linear defect that centers around the line that is defined along the end of the extra half-plane of atoms.

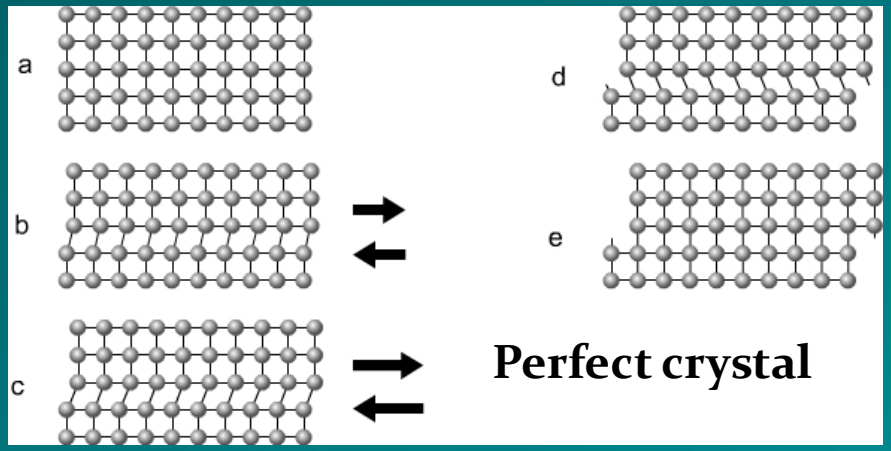


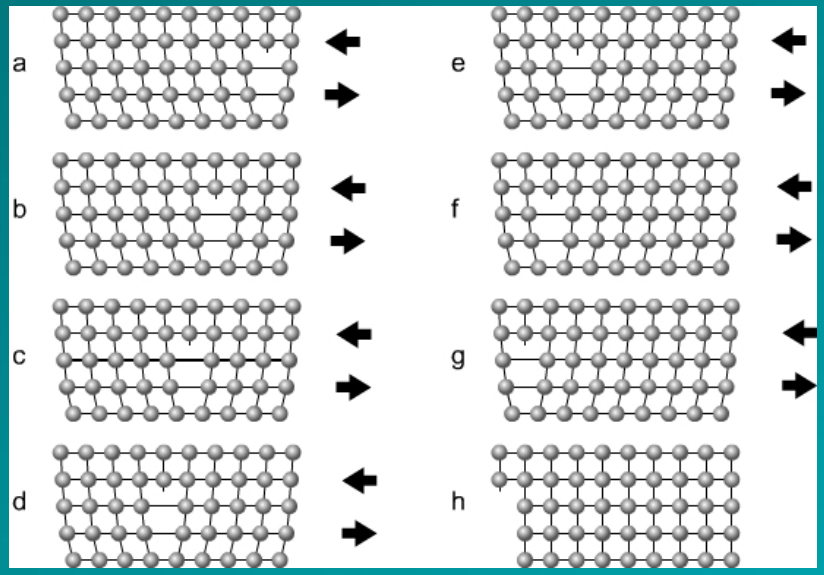






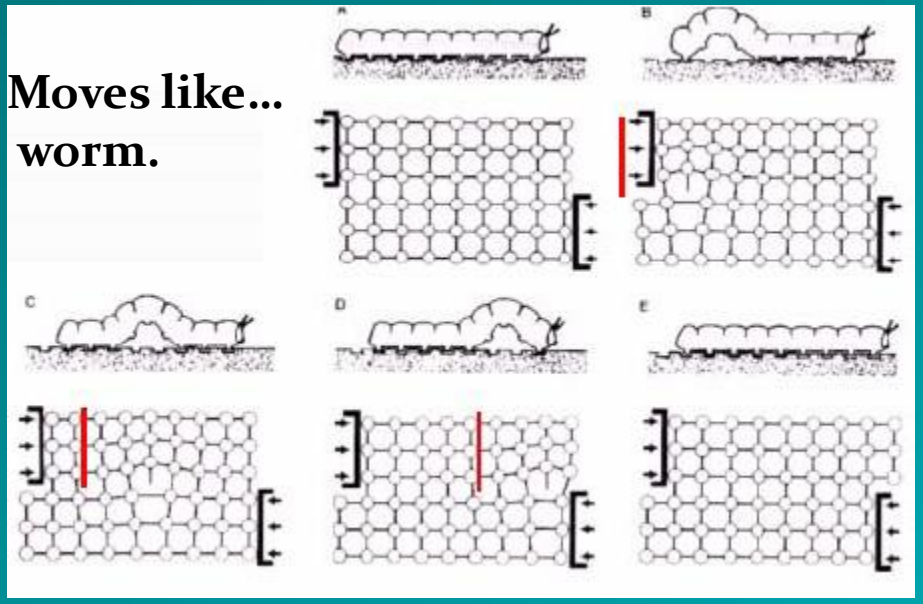
Linear defects (1D)





Real crystal

Moves like… worm.

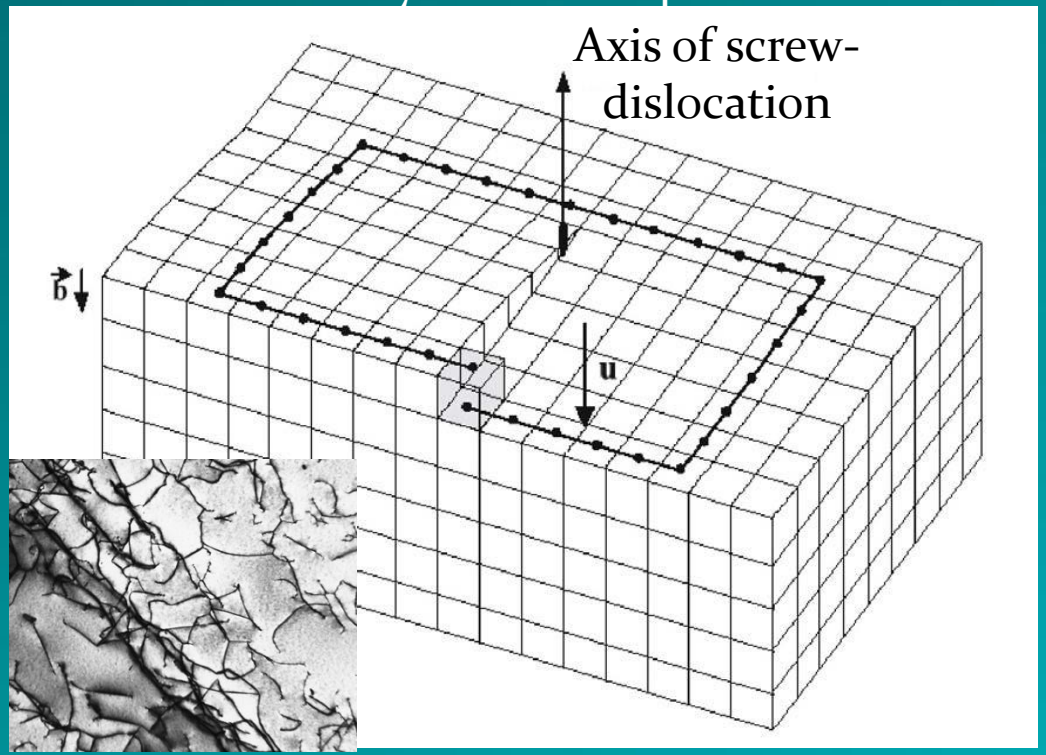


The edge dislocation line is perpendicular to the plane of the page.

The atoms above the dislocation line are squeezed together, and those below are pulled apart (Cottrell atmosphere); this is reflected in the slight curvature for the vertical planes of atoms as they bend around this extra half-plane.

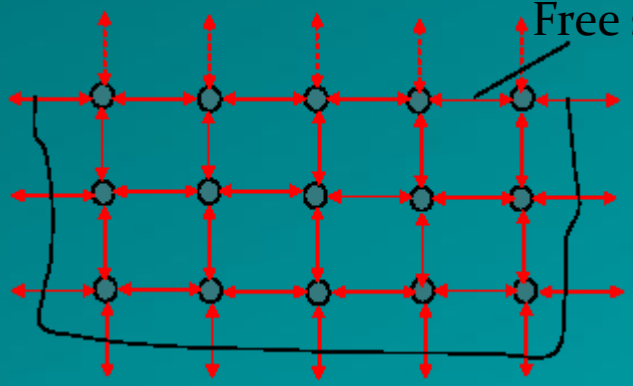
Linear defects (1D)

Another type of dislocation, called a screw dislocation, exists, which may be thought of as being formed by a shear stress that is applied to produce the distortion the left side region of the crystal is shifted one atomic distance to up relative to the right portion. The atomic distortion associated with a screw dislocation is also linear and along a dislocation line. The screw dislocation derives its name from the spiral or helical path or ramp that is traced around the dislocation line by the atomic planes of atoms.

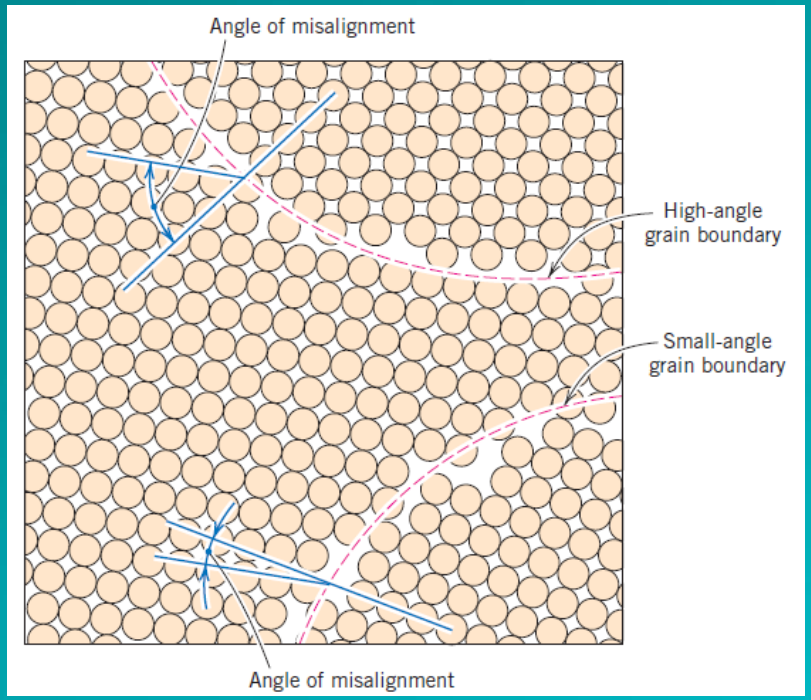


Surface defects (2D)

External surface:
Surface atoms are not bonded to the maximum number of nearest neighbors, and are therefore in a higher energy state than the atoms at interior positions. To reduce this energy, materials tend to minimize the total surface area. For example, liquids assume a shape having a minimum area—the droplets become spherical. On solid surfaces are growing up oxide-layers, chemical reactions.

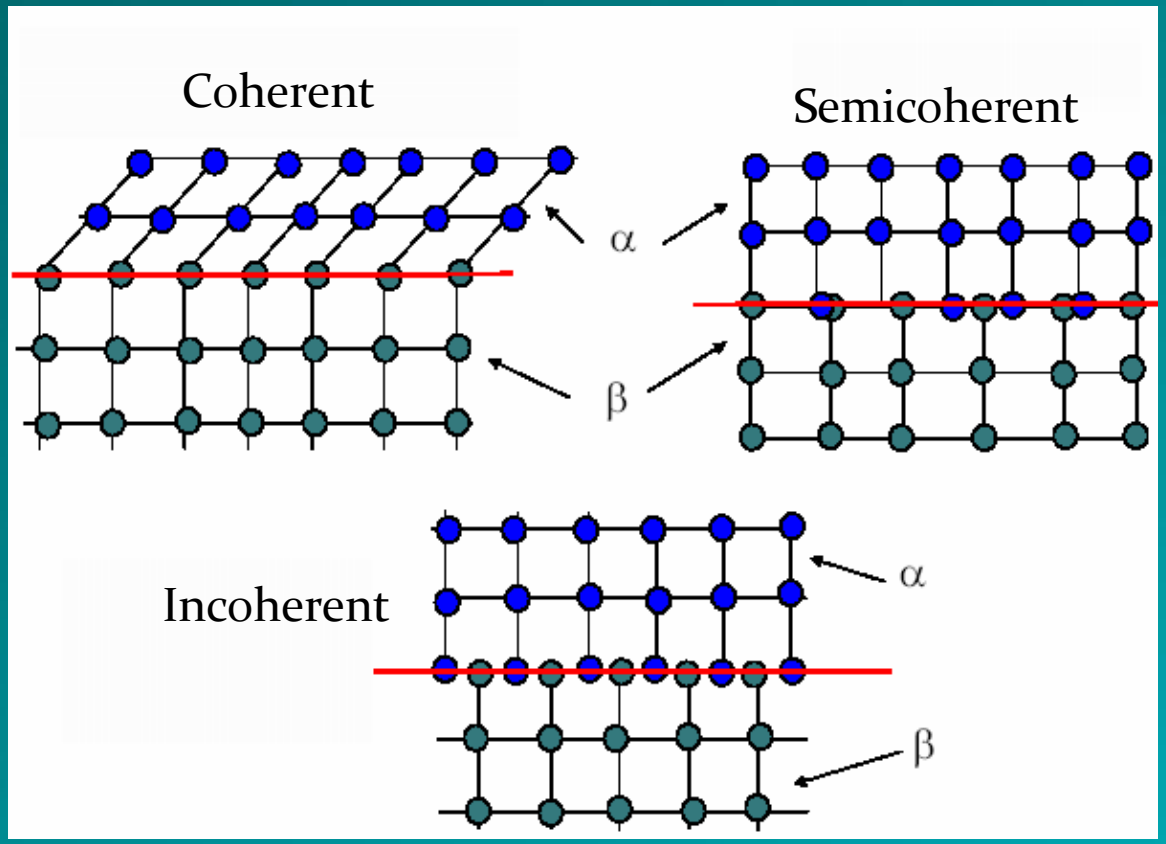


Small-angle and high-angle grain boundary:
the boundary separating two small grains or crystals having different crystallographic orientations in polycrystalline materials. Various degrees of crystallographic misalignment between adjacent grains are possible.



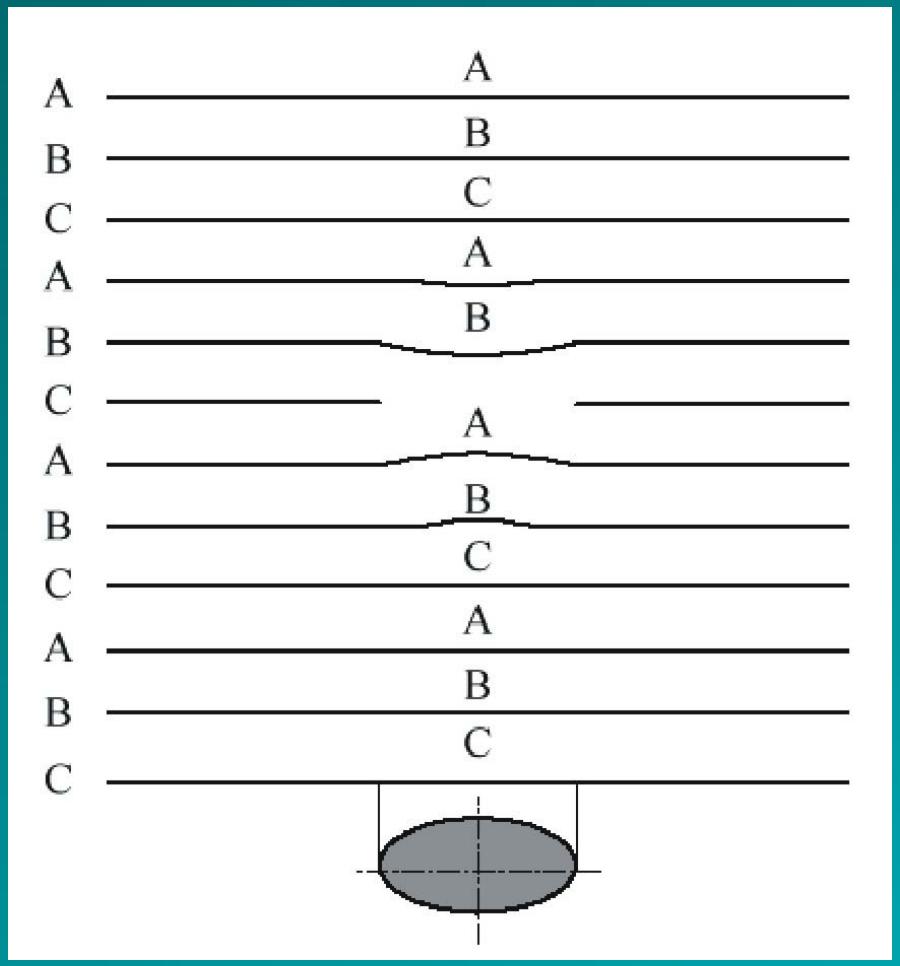
Surface defects (2D)

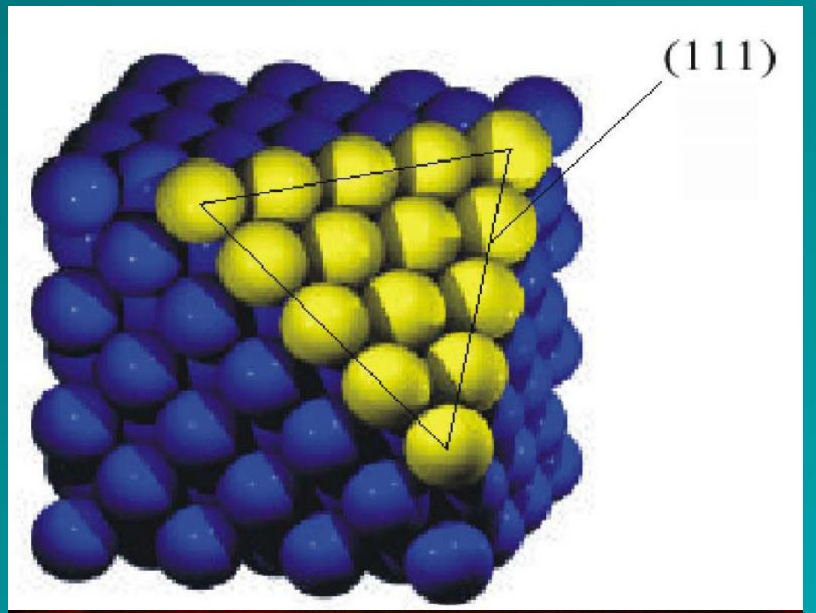
Phase boundary:
In the physical sciences, a **phase** is a region of space (a thermodynamic system), throughout which all physical properties of a material are essentially uniform.



Surface defects (2D)

Layering defects:
The order of the atomic layers are changed.

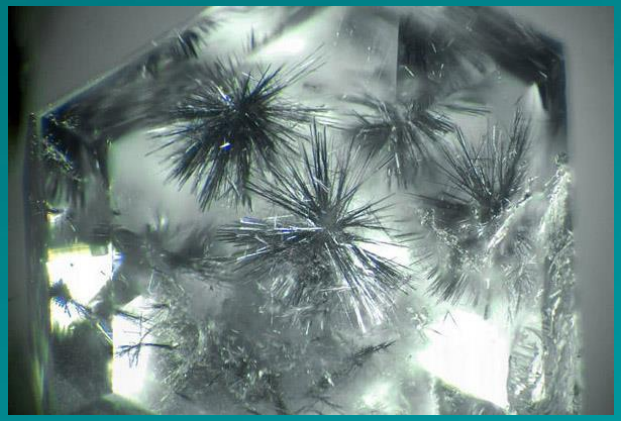


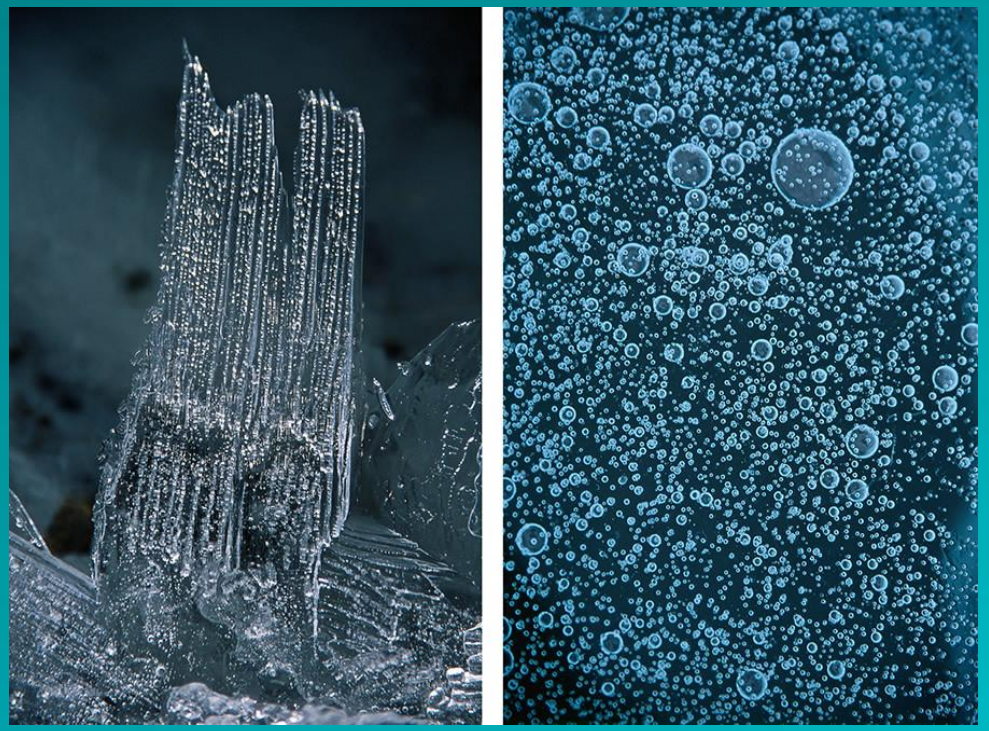


Bulk defects (3D)

Voids:
Voids are small regions where there are no atoms, and can be thought of as clusters of vacancies.

Inclusions, Precipitates:
Impurities can cluster together to form small regions of a different phase. These are often called precipitates.





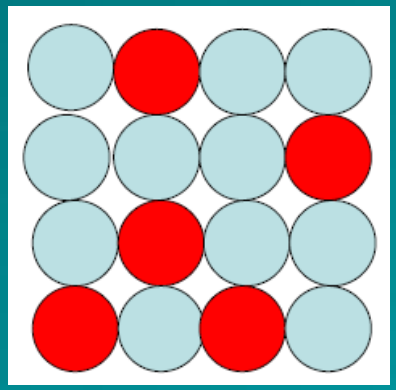
Materials Science and Engineering

Alloys, phase diagrams

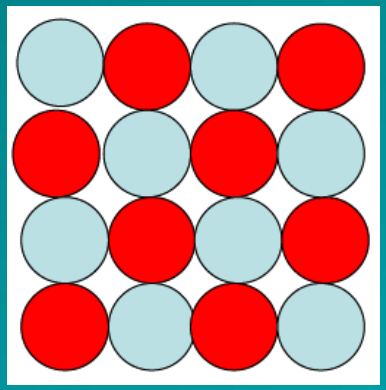
Definitions

An **alloy** is a mixture or metallic solid solution composed of two or more elements.

A **solid solution** is a solid-state solution of one or more solutes in a solvent. Such a mixture is considered a solution rather than a compound when the crystal structure of the solvent remains unchanged by addition of the solutes, and when the mixture remains in a single homogeneous phase. The solute may incorporate into the solvent crystal lattice substitutionally, by replacing a solvent particle in the lattice, or interstitially, by fitting into the space between solvent particles.



Disordered



Ordered

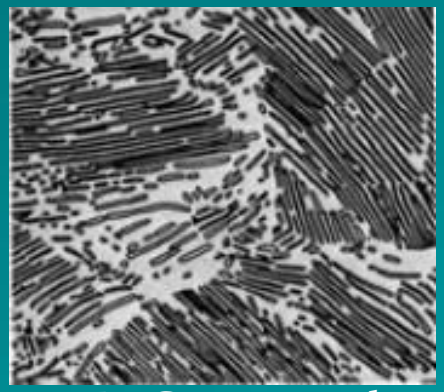
Substitutional solid solution with unlimited solubility

Structural Constituent of the micro-structure of an alloy characterized by a homogeneous average chemical composition and a uniform distribution and shape of the grains forming the constituent of the alloy's phases. The microstructure can be made up of one or more such constituents.

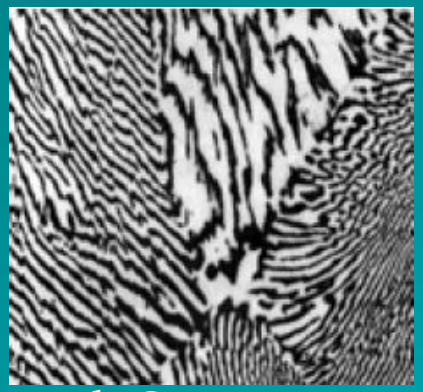
Definitions

Intermetallic compound, any of a class of substances composed of definite proportions of two or more elemental metals, rather than continuously variable proportions. The crystal structures and the properties of intermetallic compounds often differ markedly from those of their constituents.

A **eutectic system** is a mixture of chemical compounds or elements that has a single chemical composition that solidifies at a lower temperature than any other composition made up of the same ingredients (it is exist when no chance to form solid solution and intermetallic compound). Similar structure is the eutectoid in solid-solid system.



Fe-C eutectoid

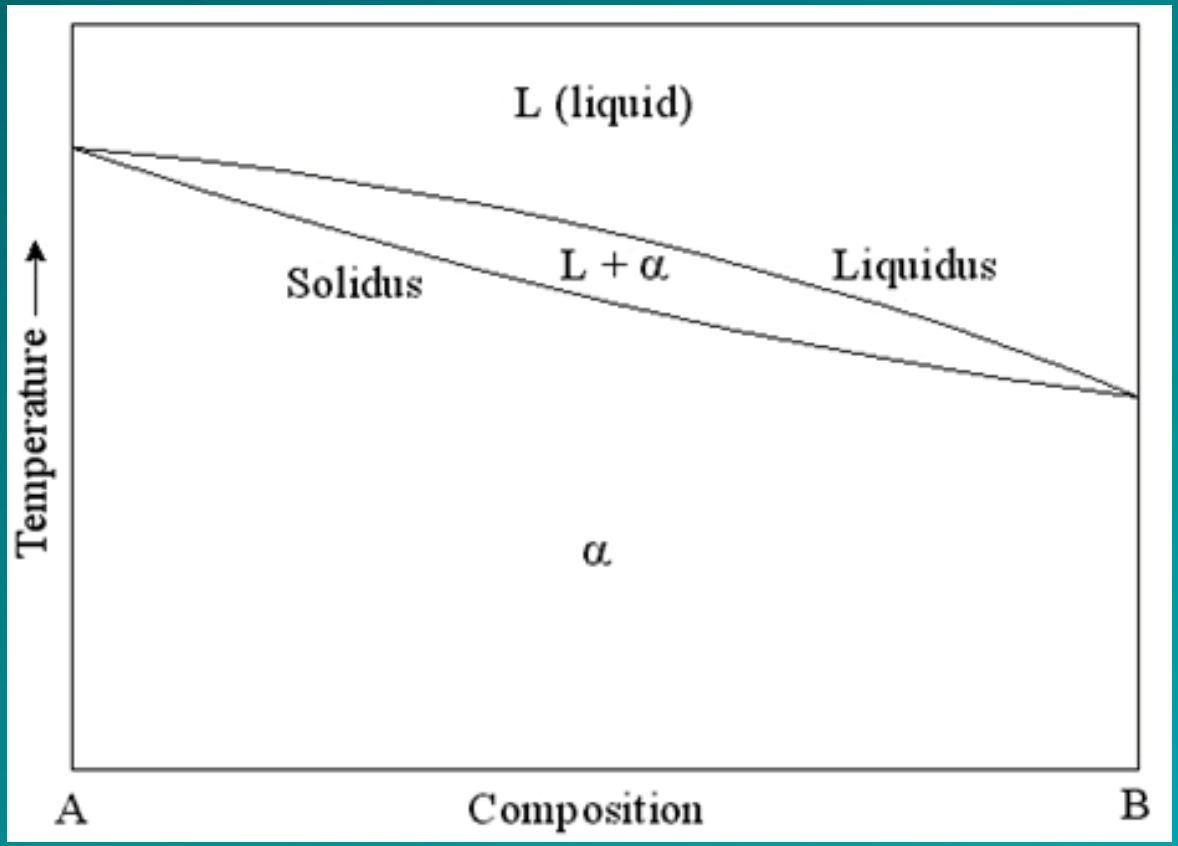


Pb-Sn eutectic

A **phase diagram** is a type of chart used to show conditions at which thermodynamically distinct phases can occur at equilibrium.

Definitions

Binary phase diagram of two components (unlimited solubility)

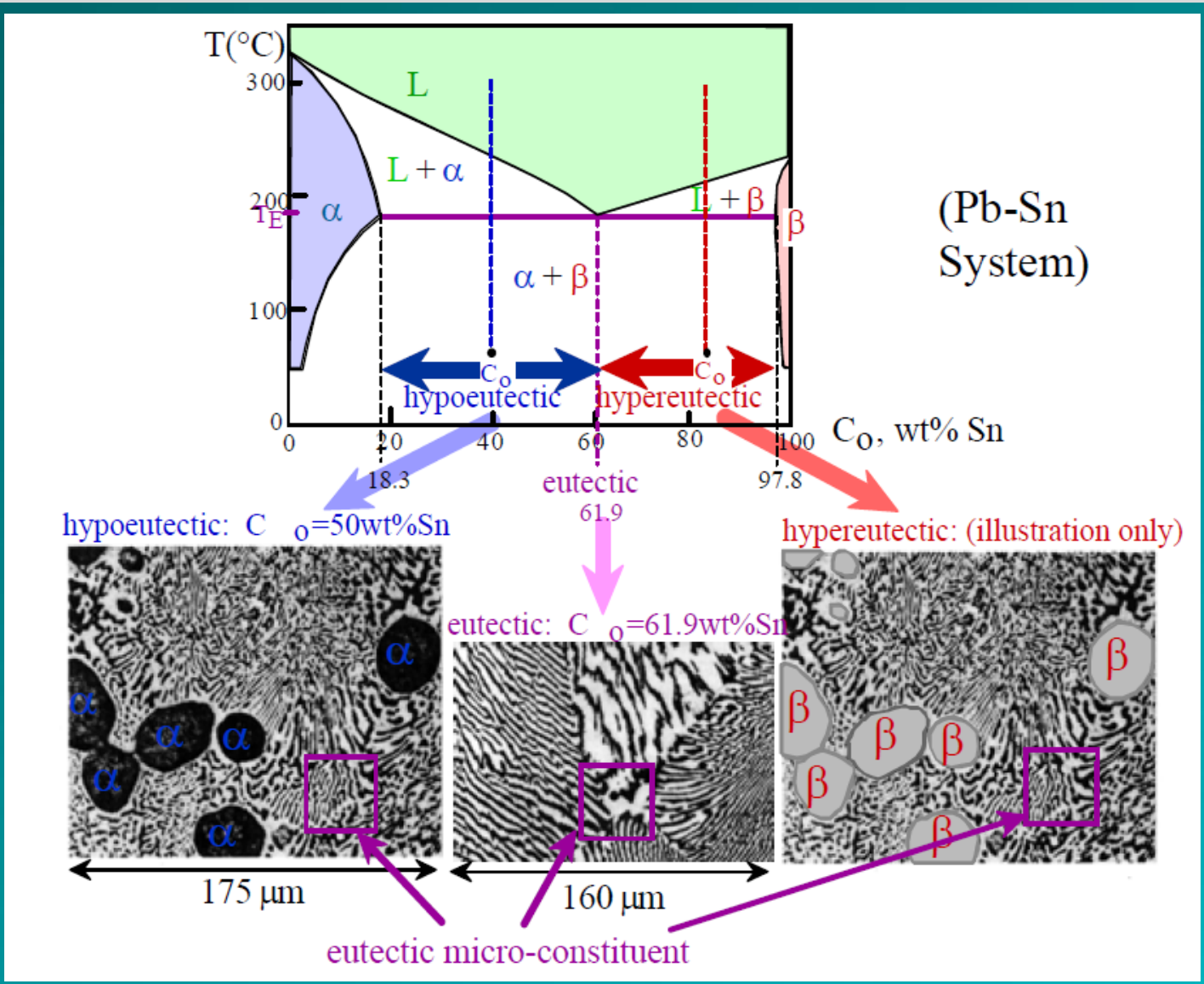


Solidus is the highest temperature at which a metal is completely solid.

The liquidus temperature specifies the maximum temperature at which crystals can co-exist with the melt in thermodynamic equilibrium. Above the liquidus temperature the material is homogeneous. Below the liquidus temperature more and more crystals begin to form in the melt.

The crystal phase that crystallizes first on cooling a substance to its liquidus temperature is termed primary phase.

Lead-tin binary phase diagram



Strengthening: allotropic transformation

Fe-C binary phase diagram