

## MATERIALOPAEDIA

An Alphabetical List of Definitions and Concepts relevant to course *Introduction To Materials Science and Engineering*. This also gives a sort of overview of the topics discussed in the course. This is based on previous presentation of the course. In the current presentation some topics may need to be added, and some others deleted. You may earn extra credit by pointing out any mistake or suggesting topics to be included.

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**AGE HARDENING:** see *Precipitation Hardening*.

**ALLOY STEEL:** a steel containing significant amounts of alloying elements such as Ni, Cr, Mn, Co, Ti, *etc.*

**AMORPHOUS MATERIALS:** A material is called amorphous (or glassy) if the arrangement of atoms do not have any long-range order, *e.g.* ordinary window glass. See also *metallic glass*.

**ANISOTROPY:** If a material has different values for a given property (say *Young's modulus*) in different directions it is said to exhibit anisotropy. Single crystals often (though not always) show anisotropy for most of their properties such as thermal expansion coefficient, electrical and thermal conductivity, diffusion coefficient, yield stress, *etc.*

**ANNEALING:**

- 1 (*of steels*) The process of austenitizing a steel followed by very slow cooling (usually obtained in a furnace which has been switched off) to produce coarse pearlite in the final microstructure is called annealing. It renders the steel very soft and ductile.
- 2 (*of metals and alloys*) A process of heating the material after cold working to remove wholly or partially the effects of cold working, *e.g.* strain hardening. At the microstructural level annealing proceeds in three stages: recovery, recrystallization and grain growth.

*Recovery:* The set of processes by which the properties of a cold worked material changes during annealing without any obvious change in the optical microstructure is called recovery. It involves reduction of vacancy concentration, annihilation of positive and negative edge dislocations lying on the same slip plane and rearrangement of edge dislocation of the same sign one above the other to form what is called a low-angle tilt boundary.

*Recrystallization:* Formation of a set of new strain-free crystals during annealing in the matrix of strained crystal of a cold-worked sample is called recrystallization. The recrystallized grains have a lower dislocation density than the strained crystal from which they form. Thus the driving force for recrystallization is the reduction in strain energy of the crystal associated with dislocations.

*Grain Growth:* A mechanism by which average grain size of a material increases to reduce the surface energy associated with grain boundaries. Thus the driving force for grain growth is the grain boundary energy.

**ASTM GRAIN SIZE NUMBER:** See *Grain Size*.

**ATACTIC:** see *Tacticity*.

**AUSTENITE:** See *Phases and Microconstituents in Steels*.

**BAINITE:** See *Phases and Microconstituents in Steels*.

**BASIS:** A synonym for *motif*, see *Crystal Structure*.

**BODY CENTRED CUBIC:** See *Cubic Bravais Lattices*.

**BOUNDARIES IN A PHASE DIAGRAM:**

*Liquidus:* A boundary between Liquid and Liquid + Solid phase fields.

*Solidus:* A boundary between solid and solid + liquid phase fields.

*Solvus:* A boundary between a single solid phase field (say  $\alpha$ ) and another field consisting of a mixture of  $\alpha$  and another solid phase  $\beta$ .

**BRAGG'S LAW:** A law that assists in the interpretation of x-ray diffraction patterns from crystalline materials. It can be stated in two parts:

*Part I:* For any diffracted beam from a crystal there exists a set of crystal lattice planes from which the diffracted beam appears to be specularly reflected, *i.e.*,

(a) the angle of incidence = angle of reflection [In contrast to the convention in optics, both angles are measured from the plane rather than the plane normal. The angle is called the Bragg angle.], and

(b) the incident beam, the diffracted beam and the normal to the lattice plane are coplanar.

*Part II.* The Bragg angle  $\theta$ , the interplanar spacing  $d$  and the wavelength  $\lambda$  satisfy the following relationship:

$$\lambda = 2 d \sin\theta .$$

Note that Bragg's law interprets a diffracted beam as a reflection from a crystal lattice plane. Because of this interpretation diffracted beams are often called reflected beams.

**BRAVAIS LATTICE:** Based on their space group symmetry lattices are classified into 14 different types. These are called the fourteen Bravais lattices. A given lattice can be described by many different unit cells. Each Bravais lattice is described by a specific unit cell known as its *conventional unit cell*. Each Bravais lattice is given the same name as its conventional unit cell. Thus face centred cubic Bravais lattice has a face centred cube as its conventional unit cell. Cf *crystal systems*.

**BRITTLE FRACTURE:** See *Fracture*.

**BRITTLENESS:** The tendency of a material to fracture without undergoing extensive plastic deformation is termed brittleness. See *Ductility*.

**BURGERS CIRCUIT:** A closed circuit joining the lattice points in a perfect crystal. If the circuit is mapped in an imperfect crystal and is pierced by a dislocation line then the circuit fails to close. The closure vector (from finish to start, say) is defined to be the burgers vector of the dislocation line.

**BURGERS VECTOR:** See Dislocations.

**CARBON NANOTUBE:** A form of carbon which can be thought of as a rolled-up graphene sheet. The structure of a nanotube is described by its chiral vector or wrapping vector  $\mathbf{C}$ . The chiral vector  $\mathbf{C}$  is a lattice translation vector in the unfolded graphene sheet such that when the sheet is folded to make the tube it wraps the perimeter of the tube. Thus the length  $C = |\mathbf{C}|$  of the chiral vector is  $\pi D$  where  $D$  is the diameter of the

tube. Since  $\mathbf{C}$  is a lattice translation vector of the graphene sheet, it can be expressed as an integer linear combination of two shortest primitive translation vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  at  $60^\circ$ . Thus  $\mathbf{C} = n \mathbf{a}_1 + m \mathbf{a}_2$  where  $n$  and  $m$  are integers. By convention a nanotube is represented by the components of its chiral vector  $(n, m)$ . Due to the rotational and reflection symmetry of the graphene sheet one can represent all distinct carbon nanotubes with  $n \geq m \geq 0$ . A tube with  $n=0$ , i.e., an  $(n,0)$  tube, is called a zig-zag tube. A tube with  $m=n$ , i.e., an  $(n,n)$  tube is called an armchair tube. A tube that is neither zig-zag nor armchair is called a chiral tube. Both zig-zag and armchair tubes have axial and transverse mirror planes and thus do not have handedness. A chiral tube lacks any mirror plane and so has left and right handed variety.

**CASE HARDENING:** A method of hardening steel by changing the composition of the surface by diffusion. It is usually done by increasing the carbon concentration (carburization) or by introducing nitrogen (nitriding) in the surface of the steel.

**CAST IRON:** Alloys Fe and C containing more than 2 wt% C are termed cast irons.

**CEMENTITE:** See *Phases and Microconstituents in Steels*.

**CHIRAL MOLECULE:** A molecule which can occur as left or right handed. Chiral molecules lack any mirror plane of symmetry.

**CHIRAL VECTOR:** A vector in the graphene sheet which determines the structure and diameter of a carbon nanotube. Also known as wrapping vector.

**CLIMB:** See *Motion of a Dislocation*.

**CLOSE-PACKED CRYSTAL STRUCTURES:** Crystal structures of some elements can be described as close packing of identical spherical atoms. These crystal structures are known as close packed structures. Two most common close packed structures are cubic close-packed (ccp) and hexagonal close-packed (hcp). Monatomic body centred cubic structure, although not strictly close-packed, also has a high packing efficiency. See *Crystal Structures*.

**CNT:** Carbon nanotube.

**COLD WORKING:** Plastic deformation of a material below its recrystallization temperature is called cold working. It leads to *strain hardening*.

**COMPOSITE MATERIALS:** A material made by intentionally mixing two or more different phases is called a composite material.

**CONFORMATION:** Various shapes a polymer chain can acquire due to rotational freedom about C-C single bonds.

**CONVENTIONAL UNIT CELL:** A specific unit cell (out of infinitely many possible ones) selected by convention to represent a Bravais lattice is called its conventional unit cell. It is usually the smallest cell which represents most of the point symmetry elements of the lattice.

**COORDINATION NUMBER:** The number of atoms closest to a given atom or site is called its coordination number.

**COORDINATION POLYHEDRON:** Polyhedron defined by the centres of nearest neighbours. For CCP and HCP structures these are cuboctahedron and twisted cuboctahedron respectively.

**CREEP:** Time dependent plastic deformation of a material at a fixed load or stress is called creep. It becomes significant at temperatures higher than 0.4 to 0.5  $T_m$ , where  $T_m$  is the melting point or liquidus temperature in K. Creep takes place mainly by three mechanisms listed below:

*Dislocation Creep:* In this mechanism the edge dislocations are able to overcome obstacles on a given slip plane by climbing up or down to a different but parallel slip plane.

*Diffusion Creep:* Creep involving diffusion of vacancies away from grain boundaries perpendicular to the stress axis to boundaries parallel to the stress axis is called diffusion creep.

*Grain Boundary Sliding:* This mechanism involves sliding of an entire grain over another grain along their common grain boundary.

**CRITICAL RESOLVED SHEAR STRESS:** See *Resolved Shear Stress*

**CROSS-SLIP:** See *Motion of a Dislocation*.

**CRYSTAL COORDINATE SYSTEM:** Any three non coplanar translation vectors **a**, **b**, and **c** of a lattice define a coordinate system which is called a crystal coordinate system. The vectors **a**, **b**, and **c** also define a parallelepiped which is a unit cell of the crystal. If vectors **a**, **b**, and **c** are selected in a manner so that any lattice translation vector **T** can be expressed as integral combination of **a**, **b** and **c**, *i.e.*,

$$\mathbf{T} = l\mathbf{a} + m\mathbf{b} + n\mathbf{c}$$

where  $l$ ,  $m$ , and  $n$  are integers then the **a**, **b**, and **c** are said to be a primitive set of basis vectors and the associated unit cell is called a primitive unit cell. If the vectors **a**, **b**, and **c** are so selected that some of the lattice translation vectors **T** require fractional values of  $l$ ,  $m$ ,  $n$  then the set of vectors and the associated unit cell is called non-primitive.

**CRYSTAL STRUCTURE:** The structure of a crystal is described in terms of lattice and motif. **Lattice** is an infinite set of discrete points such that each point has an identical neighbourhood. Lattice is not crystal as it is only a set of geometrical points. To obtain a crystal we associate with each lattice point an identical atom or a group of atoms. The atom or the group of atom associated with each lattice point is called the **motif** or **basis**. Thus to completely describe a crystal structure both lattice and motif should be given. To express this point concisely one often writes

$$\text{Crystal Structure} = \text{Lattice} + \text{Motif}$$

Some simple crystal structures are described in the table below:

Crystal Structure	Lattice	Motif	Examples
Monatomic Body Centred Cubic	BCC or Cubic I	000	$\alpha$ -Fe, Cr, K, Na
Cubic Close Packed (CCP)	FCC or Cubic F	000	$\gamma$ -Fe, Cu, Ag, Au, Al, Ni
Diamond Cubic	Cubic F	000; $\frac{111}{444}$	Diamond, Si
Zinc Blende (ZnS)	Cubic F	Zn:000; S: $\frac{111}{444}$	ZnS, SiC, GaAs,
Sodium Chloride (NaCl)	Cubic F	Na: $00\frac{1}{2}$ ; Cl: 000	NaCl, LiF, MgO

Caesium Chloride (CsCl)	Cubic P	Cs: 000; Cl: $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	CsCl ordered $\beta$ -brass
Hexagonal Close Packed (HCP)	Hexagonal P	000; $\frac{2}{3} \frac{1}{3} \frac{1}{3}$	Zn, Mg, Co, Cd

**NOTE:** Monatomic bcc structure is often called simply bcc. Similarly, CCP structure is also commonly called FCC. However, strictly speaking, both the terms BCC and FCC refer to the Bravais lattices and not the crystal structure.

**CRYSTAL SYSTEM:** Based on their *point group symmetry* (i.e., ignoring translational symmetry) lattices can be classified into seven different types. These are called the seven crystal systems. Cf. *Bravais Lattice*.

Crystal Family	Symbol	Crystal system	Characteristic Symmetry	Conventional Unit Cell Shape	Bravais Lattice
Triclinic	$a$	Triclinic	None	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$	$aP$
Monoclinic	$m$	Monoclinic	A single twofold axis	(i) Unique axis $b$ $\alpha = \gamma = 90^\circ$	$mP, mS$ ( $mC, mA$ )
				(i) Unique axis $c$ $\alpha = \gamma = 90^\circ$	$mP, mS$ ( $mA, mB$ )
Orthorhombic	$o$	Orthorhombic	Three twofold axes	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$oP, oI, oF,$ $oS$ ( $oA, oB,$ $oC$ )
Tetragonal	$t$	Tetragonal	A single fourfold axis	$a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	$tP, tI$
Hexagonal	$h$	Trigonal	A single threefold axis	(i) Rhombohedral cell $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	$hR$
				(ii) Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	
		Hexagonal	A sixfold axis	Hexagonal cell $a = b \neq c$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	$hP$
Cubic	$c$	Cubic	Four threefold axes	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	$cP, cI, cF$

P: Primitive, I: Body-centred, F: Face-centred, S (A, B, or C): End-centred or Base-centred

**CUBIC BRAVAIS LATTICES:** There are three cubic Bravais lattices: simple cubic (or cubic P), body centred cubic (or cubic I) and face centred cubic (cubic F). The conventional unit cell of a simple cubic lattice has lattice points only at the corners of a cube, that of a body centred lattice has lattice points at the corners as well as

one at the centre of the cube and the unit cell of the face centred cubic lattice has lattice points at the corners as well as at the centres of each of the cube faces.

**CUBOCTAHEDRON:** An Archimedean solid with 12 vertices, 8 triangular and 6 square faces which is *coordination polyhedron* of CCP crystal.

**CZOCHELSKI'S METHOD:** A method to grow single crystals, particularly of Si for semiconductor applications.

**DEGREES OF FREEDOM:** The number of thermodynamic variables that can be independently specified without any change in the number or identity of phases in equilibrium in a given system is called its degrees of freedom. See *Gibbs Phase Rule*.

**DIAMOND CUBIC STRUCTURE:** See *Crystal Structure*.

**DIFFUSIONAL CREEP:** See *Creep*.

**DISLOCATIONS:** A dislocation is a line defect in a crystal. It can be considered as a boundary between slip and no-slip regions on a slip plane.

A vector that characterizes the magnitude and direction of the slip distortion associated with a dislocation line is called the **Burger's vector,  $\mathbf{b}$** . The magnitude of the Burgers vector and the line along which it lies is uniquely determined. However, its sense along this line is not uniquely determined and has to be fixed by some agreed upon convention. See *Burgers Circuit*.

A unit vector which is tangent to the dislocation line is called its **line vector**.

Burger's vector of a given dislocation is constant throughout its length.

A dislocation can be classified on the basis of relative orientation of the Burgers vector and the line vector.

If the Burger's vector is perpendicular to the line vector the dislocation is called an **edge dislocation**. It can be described as the edge of an extra half plane in the crystal.

If the Burgers vector is parallel to the line vector then the dislocation is called a **screw dislocation**. It can be described as the axis of a helical ramp of atomic planes.

If the Burger's vector is neither parallel nor perpendicular to the line vector the dislocation is called **mixed dislocation**. A mixed dislocation can be considered to have a screw and an edge component with the Burgers vector decomposed into components parallel and perpendicular to the line vector respectively.

**DISLOCATION CREEP:** See *Creep*.

**DISLOCATION DENSITY:** The length of dislocation per unit volume of a sample or the number of dislocations crossing unit area of a test surface in the sample is called its dislocation density and can be expressed in units of  $\text{m}^{-2}$ .

**DISLOCATION NODE:** A point where more than one dislocation meet is called a node. If all the vectors either point into the node or out of it then the sum of the Burgers vectors of all the dislocations meeting at the node is zero:

$$\sum \mathbf{b}_i = 0$$

This is known as Frank's rule.

**DISPERSION STRENGTHENING:** Strengthening obtained by dispersing insoluble particles of a second phase in a matrix. An example is thoria-dispersed nickel (TD

Ni) where the ThO<sub>2</sub> particles are dispersed in the matrix of Ni to give a material stronger than Ni. The mechanism of hardening is similar to precipitation hardening, the difference being that the strengthening particles are not a result of phase transformation but are mechanically mixed.

**DUCTILE FRACTURE:** See *Fracture*.

**EDGE DISLOCATIONS:** See *Dislocations*.

**DUCTILITY:** Ability of a material to undergo extensive plastic deformation before fracture is called ductility. See *Brittleness*.

**EUTECTIC REACTION:** See *Invariant Reactions*.

**EUTECTOID REACTIONS:** See *Invariant Reactions*.

**FACE CENTRED CUBIC:** See *Cubic Bravais Lattice*

**FERRITE:** See *Phases and Microconstituents in Steels*.

**FRACTURE:** Separation of an object in two or more pieces due to mechanical loading is termed fracture. It is generally classified as brittle or ductile.

**Brittle Fracture:** A fracture following negligible amount of macroscopic plastic deformation is termed brittle fracture.

**Ductile Fracture:** A fracture preceded by extensive macroscopic plastic deformation of the material is called a ductile fracture.

**FRANK-READ SOURCE:** A mechanism by which a dislocation pinned at two points on a slip plane can continuously generate new dislocation loops under the application of a shear stress parallel to the slip plane. There is a minimum value of shear stress required to operate a Frank-Read source given by

$$\tau = \frac{\mu b}{l}$$

where  $\mu$  is the shear modulus of the material,  $b$  the Burgers vector of the dislocation line and  $l$  is the distance between the pinning points.

**FRANK'S RULE:** See *Dislocation Nodes*.

**FULLERENE:** A cage like molecule C<sub>60</sub> of 60 carbon atoms. Each carbon atom is bonded to three other atoms. They form hexagonal and pentagonal rings of C-C bonds. The carbon atoms are located at the vertices of a truncated icosahedrons which has 12 pentagons and 20 hexagons. There are other fullerenes also with  $n$  atoms where  $n$  is 20, 70, 100 etc. A fullerene C <sub>$n$</sub>  for any  $n$  always has 12 pentagons, a result which follows from Euler polyhedron formula. The number of hexagons depend upon  $n$ .

**GIBBS PHASE RULE:** If  $P$  is the number of phases and  $C$  the number of components in a system at equilibrium then the number of degrees of freedom  $F$  is given by

$$F = C - P + 2.$$

In a binary diagram where pressure is held constant degrees of freedom reduce by one and the phase rule takes the form

$$F = C - P + 1 \text{ (Pressure held constant).}$$

**GLASS:** a synonym for an amorphous material. See *amorphous material*.

**GRAINS:** See Polycrystals.

**GRAIN BOUNDARY:** If two crystals of the same phase are related to each other by a rotation then the boundary between them is called a grain boundary. If the rotation axis lies in the plane of the boundary it is called a tilt boundary. If the rotation axis lies perpendicular to the boundary plane then the boundary is called a twist boundary. For a more general orientation of the axis with respect to the boundary plane we have general grain boundaries. See also Interfaces.

**GRAIN BOUNDARY SLIDING:** See *Creep*.

**GRAIN GROWTH:** See *Annealing*.

**GRAIN SIZE:**

There are two common ways of specifying grain size:

1. **MEAN INTERCEPT SIZE:** If  $N$  grain boundaries intersect on a line of length  $L$  drawn on a microstructure of magnification  $M$  then the mean intercept grain size is defined by

$$l = \frac{L}{NM}.$$

2. **ASTM GRAIN SIZE NUMBER** If the number of grains seen in a sample at 100X magnification in an area of an inch squared is  $n$  then the ASTM grain size number  $N$  is defined through the relation

$$n = 2^{N-1}$$

**GRAIN SIZE STRENGTHENING:** Grain boundaries obstruct the motion of a dislocation thus causing strengthening. Smaller the grain size, more is the total grain boundary area in a sample of given volume and thus more is the strengthening. This is expressed quantitatively through the **Hall-Petch relationship**, a relationship relating the yield strength  $\sigma_y$  of a crystal to its average grain size  $d$ :

$$\sigma_y = \sigma_y^0 + \frac{k}{\sqrt{d}}.$$

Here  $\sigma_y^0$  and  $k$  are constants.  $\sigma_y^0$  can be considered to be the yield stress of a large single crystal.

**GRAPHENE:** A 2D form of carbon in which each carbon is  $sp^2$  hybridized to form bonds with three nearest neighbours. The bond angles are  $120^\circ$  and the C atoms arrange themselves on the vertices of a tiling of regular hexagons.

**GRIFFITH'S CRITERION:** A criterion specifying a critical tensile stress which will cause fracture in a brittle solid containing cracks. It is written as:

$$\sigma_f = \left( \frac{2E\gamma}{\pi c} \right)^{\frac{1}{2}}$$

where  $\sigma_f$  is the fracture stress,  $E$  is the Young's modulus and  $\gamma$  is the surface energy of the material.

**HALL-PETCH RELATIONSHIP:** See Grain Size Strengthening.



**HARDENABILITY:** A measure of ease with which a steel can be hardened by quenching. Slower is the critical cooling rate to obtain martensite, higher is the hardenability. Alloy steels have higher hardenability than plain carbon steels.

**HARDNESS:** The resistance to plastic deformation of a material as measured by indenting a well-polished surface by a standard indenter under a standard load.

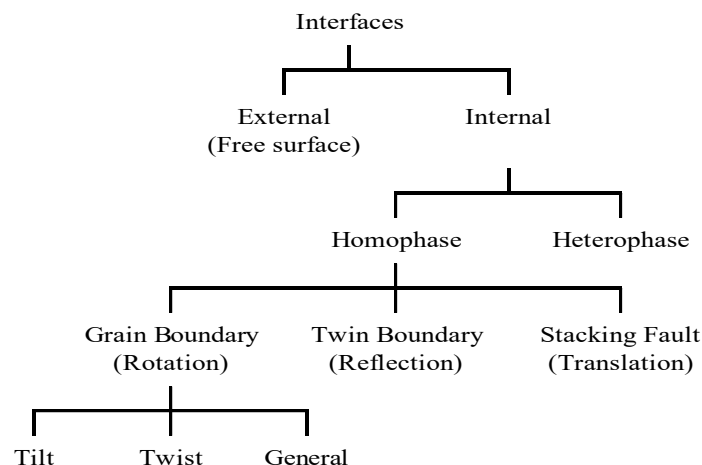
**HEXAGONAL CLOSE PACKED CRYSTAL:** See *Close Packed Crystal Structures*.

**HOT WORKING:** Plastic deformation of a material above its recrystallization temperature is called hot working.

**HUME-ROTHERY RULES:** Some binary systems (e.g., Cu-Ni) show complete solid solubility, i.e., the two components can dissolve in each other in any proportion to give a single phase solid solution. However, such complete solid solubility is seen only in a very limited number of binary systems. Hume-Rothery rules are empirical criteria to identify which systems would show complete solubility and which will not. There are four Hume-Rothery rules:

1. The sizes of the two atoms should not be similar, roughly within 15% of each other.
2. The crystal structure of the two elements should be the same.
3. The electronegativity of the two elements should not be very different.
4. The valences of the two elements should be the same.

**INTERFACES:** Boundary between two phases or two crystals of the same phase is an interface. A possible classification is shown below



**INTERPLANAR SPACING,  $d_{hkl}$ :** For any value of Miller indices (hkl) one can construct a plane which has intercepts  $a/h$ ,  $b/k$  and  $c/l$  on the three crystallographic axes.

**INTERSTITIAL SOLID SOLUTION:** See *Solid Solution*.

**INTERSTITIAL VOIDS:** Empty spaces left between atoms of a crystal. In close packed crystals there are two important kinds of voids called the tetrahedral and octahedral voids. An atom in any given layer touches three atoms in the adjacent layer. Centres of these four atoms are at the corners of a regular tetrahedron. The central space between these four atoms is called a **tetrahedral void**. To define an octahedral void

consider two adjacent close packed layers say A and B. Then the C type sites in either of the layers are unoccupied. Consider two such C sites one above the other (one in A layer and the other in B layer). The C sites in either layer are surrounded by three atoms. The centres of the three A atoms and the three B atoms which surround these C sites are at the vertices of a regular octahedron. The central space between these six atoms is called the **octahedral void**.

It is possible to define tetrahedral and octahedral voids in a monatomic bcc structure, which is not strictly close packed. But in this case the tetrahedron or the octahedron is not regular but distorted.

Voids can accommodate smaller atoms to give compounds or interstitial solid solutions. The ratio of radius  $r$  of largest atom that can fit in a void defined by atoms of radius  $R$  characterizes the size of the void. This and some other properties of the voids in a close-packed structure (CCP or HCP) are given below.

CCP or HCP structures	Coordination Number (No. of atoms surrounding the void)	Effective number of voids per atom in the structure	$r/R$
Tetrahedral Void	4	2	$(\sqrt{3}/\sqrt{2}) - 1 \approx 0.225$
Octahedral Void	6	1	$\sqrt{2} - 1 \approx 0.414$

Voids are also important in monatomic BCC structure. Here we have irregular tetrahedral and octahedral voids. The number of voids per atom and the  $r/R$  ratio for this structure are given in the table below

Monatomic BCC structure	Coordination Number (No. of atoms surrounding the void)	Effective number of voids per atom in the structure	$r/R$
Irregular Tetrahedral Void	4	12	$\frac{\sqrt{5}}{\sqrt{3}} - 1 = 0.291$
Irregular Octahedral Void	6	6	$\frac{2}{\sqrt{3}} - 1 = 0.155$

**ISOTACTIC:** see Tacticity.

**INVARIANT REACTIONS:** In a binary phase diagram phase reaction occurring at a fixed temperature and fixed compositions of all the phases involved are called invariant reactions (the degree of freedom for equilibrium represented by the reaction is zero). Four important invariant reactions in a binary diagram are listed below ( $L$  represents a liquid phase whereas  $\alpha$ ,  $\beta$  and  $\gamma$  represent different solid phases):

Eutectic reaction:  $L \xrightarrow{\text{cool}} \alpha + \beta$

Eutectoid reaction:  $\gamma \xrightarrow{\text{cool}} \alpha + \beta$

Peritectic reaction:  $L + \alpha \xrightarrow{\text{cool}} \beta$

Peritectoid reaction:  $\alpha + \beta \xrightarrow{\text{cool}} \gamma$

**LATTICE:** See *Crystal Structure*.

**LATTICE PARAMETERS:** A lattice can be described in terms of a properly selected parallelepiped unit cell. The unit cell itself is defined in terms of three lattice translation vectors **a**, **b** and **c**. The magnitudes of these vector and the three interaxial angles between them are called the lattice parameters. Commonly these parameters are given symbols *a*, *b*, and *c* for the lengths of **a**, **b** and **c** respectively, and  $\alpha$ ,  $\beta$  and  $\gamma$  for the angles between **b** and **c**, **c** and **a**, and **a** and **b** respectively. Thus a lattice can be described in terms of any of these equivalent ways: (i) by giving its unit cell, or (ii) by giving the three lattice translation vectors **a**, **b** and **c**, or (iii) by giving the six lattice parameters *a*, *b*, *c*,  $\alpha$ ,  $\beta$  and  $\gamma$ .

**LATTICE TRANSLATION:** Any vector from a lattice point to another lattice point is called a lattice translation

**LEVER RULE:** A rule to calculate the fraction or proportion of two phases in equilibrium in terms of their compositions. If in an alloy of composition  $C_0$ ,  $\alpha$  and  $\beta$  are two phases in equilibrium with their respective proportions  $f_\alpha$  and  $f_\beta$  and their compositions  $C_\alpha$  and  $C_\beta$  then the Lever rule gives

$$f_\alpha = \frac{C_\beta - C_0}{C_\beta - C_\alpha}; \quad f_\beta = \frac{C_\alpha - C_0}{C_\alpha - C_\beta}.$$

The rule can be derived by a simple mass balance.

**LINE VECTOR:** See *Dislocations*.

**LIQUIDUS:** See *Boundaries in a Phase Diagram*.

**MARTENSITE:** See *Phases and Microconstituents in Steel*.

**METALLIC GLASS:** Metals are usually crystalline. However, they can be rendered amorphous or glassy by special techniques. Such products are known as metallic glasses. One such technique is *rapid solidification* where a liquid metal is cooled as fast as a million degrees Celsius per second. Such rapid rates of cooling are required to avoid formation of crystals. However, there are certain compositions which do not require such rapid rates of cooling. These are called Bulk Metallic Glass (BMG). One application of metallic glasses is as core material of transformers.

**MILLER INDICES:** A set of three numbers to specify planes and directions in a crystal.

**DIRECTIONS:** Let **r** be a lattice vector along the direction of interest. If

$$\mathbf{r} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}$$

where **a**, **b** and **c** are the vectors defining the unit cell of the system, then the Miller indices of the direction is given as  $[u \ v \ w]$ . We usually cancel any common factor or clear fractions to reduce *u*, *v*, and *w* to smallest integers.

**PLANES:** Select the origin of the crystal coordinate system such that it does not lie on the plane of interest (Equivalently, select a plane parallel to the given plane and not passing through the origin.). Find the intercepts on the three crystallographic axes in terms of the lattice parameters *a*, *b* and *c*, (i.e., if the actual intercepts are *x*, *y* and *z* then the intercepts in terms of *a*, *b* and *c* are *x/a*, *y/b* and *z/c* respectively). Take the reciprocal of these intercepts and cancel any common factor

or multiply by a suitable integer to get three integers h, k and l. The Miller Indices of the plane is then given as (h k l).

Note:

1. Square brackets, [...], are used for directions and parentheses, (...), for the planes.
2. The way these indices are defined, they represent not a specific direction or plane but the entire set of parallel direction and planes.

**MIXED DISLOCATIONS:** see *Dislocations*.

**MOTIF:** Synonym of *Basis*. See *Crystal Structure*.

**MOTION OF A DISLOCATION:**

*Glide:* Motion of a dislocation line on its slip plane is called glide. An edge dislocation has a specific plane defined by its line vector and Burgers vector on which it can glide. A screw dislocation can glide on any plane passing through its line. For a dislocation to glide a shear stress parallel to the slip plane in the direction of the Burger's vector is required.

*Climb:* Motion of an edge dislocation from one slip plane to a parallel slip plane. If the extra half plane associated with the dislocation shortens during this motion then the dislocation is said to climb up; if the half plane lengthens it climbs down. The climb motion involves diffusion of atoms and thus is significant at higher temperatures.

*Cross Slip:* Since the glide motion of a screw dislocation is not confined to a specific plane it can change its slip plane during its motion. Such a movement of a screw dislocation from one slip plane to another slip plane which is inclined to the original slip plane is called cross-slip. Because of glide motion of an edge dislocation is confined to a specific slip plane it cannot cross slip.

**NETWORK FORMERS:** In oxide glasses the oxides which form the three dimensional random network of the glass are called network formers, e.g.,  $\text{SiO}_2$ ,  $\text{B}_2\text{O}_3$  etc.

**NETWORK MODIFIERS:** In oxide glasses oxides which break the network of the network forming oxides, thus reducing the softening temperature of the glass, are called network modifiers, e.g.,  $\text{Na}_2\text{O}$ ,  $\text{CaO}$ .

**NORMALIZING:** The process of cooling austenitized steel in air so that the transformed product is fine pearlite is called normalizing.

**NUCLEATION:** During phase transformation, the initial formation of a stable transformed region is called nucleation. The nucleus must have a size larger than a critical size determined by the thermodynamics of the transformation.

**OCTAHEDRAL VOID:** See *Voids*.

**OVERAGING:** see *Precipitation Hardening*.

**PACKING EFFICIENCY:** The ratio of volume occupied by atoms in a unit cell to the volume of the unit cell is called its packing efficiency. This number determines the density or efficiency with which the atoms of a crystal are packed. Also called packing density or packing factor.

**PEARLITE:** See *Phases and Microconstituents in Steels*.

**PERITECTIC REACTION:** see *Invariant Reaction*.

**PERITECTOID REACTION:** see *Invariant Reaction*.

**PHASE:** A physically distinct, chemically homogeneous and mechanically separable part of a system is called phase.

**PHASE DIAGRAMS:** A diagram depicting the phase or phases existing in equilibrium as a function of thermodynamic variables is called a phase diagram. For a unary system (single-component) pressure and temperature are usually selected as thermodynamic variables. For a binary system (two-component) the variables selected are temperature and composition, with pressure being held constant.

**PHASE RULE:** See *Gibbs Phase Rule*.

**PHASES AND MICROCONSTITUENTS IN STEEL:**

**AUSTENITE:** Face centred cubic phase of iron and solid solutions based on this structure.

**BAINITE:** A two-phase microconstituent of steel containing fine needles of cementite in a matrix of ferrite. It is produced at temperatures between those at which pearlite and martensite form. In plain carbon steels it cannot be produced by continuous cooling, rather it is obtained by isothermally transforming austenite below the nose of the TTT curve. In alloy steels bainite can be obtained by continuous cooling.

**CEMENTITE:** The intermetallic compound of formula  $\text{Fe}_3\text{C}$ . It is the hardest phase present in steel.

**FERRITE:** A body-centred cubic phase of iron and solid solutions based on this phase.

**MARTENSITE:** A metastable phase of steel formed when austenite is cooled at a rate faster than a critical cooling rate. Its crystal structure is body centred tetragonal. In carbon steels the martensite is very hard and brittle.

**PEARLITE** A two-phase microconstituent of steel consisting of alternate lamellae of cementite and ferrite. It forms by eutectoid decomposition of austenite. Note that both pearlite and Bainite are mixtures of the same two phases: ferrite and cementite. However they differ in the morphology (shapes) and the distribution of the two phases.

**TEMPERED MARTENSITE:** A two-phase microconstituent of steel consisting of fine particles of *cementite* in ferrite produced as result of *tempering* of quenched martensitic steel.

**PLAIN CARBON STEEL:** Steels containing only C as an intentional alloying elements. Small amounts of Si and Mn may be present as impurities.

**POLYCRYSTAL:** An assembly of several crystals of the same phase but in different orientation is called a polycrystal and such samples are called polycrystalline. All common methods of production, e.g., casting, render the product in polycrystalline form. Individual crystals in a polycrystal are also called grains and the boundary between them grain boundaries.

**POINT GROUP SYMMETRY:** A symmetry operation which leaves at least one point invariant (unmoved) by its operation is called a point symmetry operation, e.g. rotation, reflection, inversion etc. The collection of all point symmetry operations of an object or a crystal is called its point group.

**PRIMITIVE UNIT CELL:** See Unit Cell.

**PRECIPITATION HARDENING:** A process in which strength of an alloy quenched from a high temperature to a lower temperature gradually increases with time due to precipitation of a new phase. Because hardness increases with time the process is also called age hardening. The alloy attains a peak at some time after which the hardness begins to decrease with time due to coarsening of existing precipitates, a phenomenon called overaging.

**PROEUTECTIC AND PROEUTECTOID PHASES:** If an alloy of a composition away from the eutectic composition is cooled slowly from the liquid phase then one of the two solid phases (depending upon whether the alloy composition is more or less than the eutectic composition) forms first at temperatures above the eutectic temperature. In the final microstructure this microconstituent is called the proeutectic phase. Similar interpretation for proeutectoid phase (read the above text replacing 'eutectic' by 'eutectoid' and 'liquid phase' by 'single solid phase').

**QUENCHING:** Any rapid cooling of a material from a higher temperature to a lower temperature is called quenching. For steels, the term denotes cooling from a temperature where austenite is stable to a temperature where martensite forms. The cooling has to be sufficiently rapid to avoid formation of pearlite.

**RAPID SOLIDIFICATION:** A method of cooling a liquid metal extremely fast to avoid crystallization and obtain amorphous metal or metallic glass. A cooling rate as high as  $10^6 \text{ K s}^{-1}$  has been achieved. In one common method known as melt spinning a jet of molten metal is squirted on to a rapidly spinning water cooled copper wheel giving a product in form of rapidly cooled ribbon.

**RECOVERY:** See *Annealing*.

**RECRYSTALLIZATION:** See *Annealing*

**RESIDUAL STRESS:** A stress state existing in a material in the absence of any externally applied loads. this can be harmful or beneficial. For a beneficial example, see *Tempering Of Glass*.

**RESOLVED SHEAR STRESS:** The component of applied tensile stress along the slip plane in the slip direction is called the resolved shear stress (RSS). It is given by

$$\tau_{RSS} = \sigma \cos \theta \cos \phi$$

Here,  $\tau_{RSS}$  is the resolved shear stress,  $\sigma$  is the applied tensile stress and  $\theta$  and  $\phi$  are the angles that the tensile axis make with the slip direction and the slip plane normal.

The minimum value of the resolved shear stress required to initiate slip is called the critical resolved shear stress (CRSS),  $\tau_{CRSS}$ . Since the initiation of slip on the slip plane leads to the beginning of the yielding of the crystal we can write

$$\tau_{CRSS} = \sigma_y \cos \theta \cos \phi,$$

where  $\sigma_y$  is the yield stress of the material. Since  $\tau_{CRSS}$  is constant (See Schmid's Law), but  $\theta$  and  $\phi$  depend upon the crystallographic direction of the stress axis,  $\sigma_y$  is usually different in different crystallographic direction.

*Schmid's Law.* This states that the value of critical resolved shear stress (CRSS) is a material property independent of the orientation of the tensile axis with respect to the slip system. Thus if  $\theta$  and  $\phi$  change then  $\sigma$  changes accordingly to give a constant value of the CRSS.

**SCREW DISLOCATIONS:** see *Dislocations*.

**SIMPLE CUBIC LATTICE:** see *Cubic Bravais Lattices*.

**SINGLE CRYSTAL:** A sample of a single phase material without any grain boundaries is called a single crystal. Cf. *Polycrystal*.

**SLIP:** The parallel movement of a portion of a crystal over another portion across a crystallographic plane is called slip. Slip takes place on well-defined crystallographic planes, known as slip planes, in well-defined crystallographic directions, known as slip directions. A combination of a slip direction lying in slip plane is called slip system. Slip takes place because of motion of dislocations.

**SLIP DIRECTION:** See *Slip*.

**SLIP PLANE:** See *Slip*.

**SLIP SYSTEM:** See *Slip*.

**SOLID SOLUTION:** A crystal in which some of the sites that should have been vacant (voids) are occupied by some smaller atoms or a crystal in which some of the sites are occupied by a different kind of atoms is called a solid solution. In the first case where the solute atom occupies the interstitial voids is called interstitial solid solution. In the second case where a solute atoms substitutes an atom of the host crystal from its regular site is called substitutional solid solution.

**SOLID SOLUTION STRENGTHENING:** Solute particles obstruct the motion of a dislocation moving in a crystalline solid solution. This increases the strength of the crystal.

**SOLIDUS:** See *Boundaries in a Phase Diagram*.

**SOLVUS:** See *Boundaries in a Phase Diagram*.

**SPACE GROUP SYMMETRY:** The complete symmetry of a crystal including all its point symmetries as well as translational symmetry is called its space group symmetry. Lattices can have only one of the 14 space groups. These are known as 14 Bravais lattices. A crystal (lattice+motif) can have any of 230 space groups.

**STACKING FAULT:** Close packed crystal structures consist of stacking of close packed layers of atoms in a well specified repeating sequence. For example, a cubic close packed crystal is described by a stacking sequence of ...*ABCABC*.... In such crystals some time there is a fault in the stacking sequence such that on either side of the fault plane the stacking is perfect but it does not continue through the fault plane. Such faults are known as stacking faults. As an example, consider the sequence *ABCABCAB|ABCABC*. On either side of the vertical line the sequence conforms to the ccp packing. But at the vertical line a *C* plane is missing. The vertical line represents the plane of stacking fault.

**STEREoisomerism:** Synonym of *Tacticity*.

**STRAIN HARDENING:** The increase of yield strength (and hardness) of a crystal during *cold working* is termed strain hardening. This is due mainly to the increase in dislocation density of the crystal.

**STRENGTHENING MECHANISMS:** There are four important strengthening mechanisms (mechanisms that increase their yield strength) in a crystalline alloy:

Grain Size Strengthening

Solid Solution Strengthening  
Precipitation Hardening  
Strain Hardening

Look up these topics for details

**STRESS CONCENTRATION:** The stress near a crack tip in a stressed solid is much higher than the overall nominal stress. This is called stress concentration.

**SUBSTITUTIONAL DIFFUSION:** See *Diffusion*.

**SUBSTITUTIONAL SOLID SOLUTION:** See *Solid Solution*.

**SURFACE DEFECTS:** See *Interfaces*.

**SYNDIOTACTIC:** see *Tacticity*.

**TACTICITY:** Tacticity relates to the arrangement of side groups along a polymer chain. If the side groups all occur on the same side of the chain the arrangement is called **isotactic**. If the side groups occur alternately on either side of the chain it is called **syndiotactic**. If the side groups occur on either side in a random fashion the arrangement is called **atactic**. Tacticity is also known as chain configuration or stereoisomerism. Thus isotactic, syndiotactic and atactic chains are three different chain configurations or three different stereoisomers of the same polymers. Configuration of the chain should be distinguished from its conformations. Different conformations arise due to freedom of rotation about C-C bond.

**TANGENT VECTOR:** See *Dislocations*.

**TEMPERING:**

(*of steels*): Heating of a quenched steel with martensitic structure to render it more ductile at the cost of some reduction in strength is called tempering. This occurs due to transformation of martensite to a mixture of ferrite and cementite known as tempered martensite. In tempered martensite cementite forms as extremely small particles dispersed in a continuous matrix of ferrite.

(*of glasses*): A process to introduce residual compressive stresses in the surface of glass by heating the glass above its softening temperature and then cooling the surface by jets of air.

**TEMPERED MARTENSITE:** See Tempering of Steels.

**TETRAHEDRAL VOID:** See Voids.

**TIE LINE RULE:** A rule to find the equilibrium composition of phases in a two phase mixture of a binary alloy. At the temperature concerned draw a horizontal (isothermal) line in the two-phase region terminating at the phase boundaries. This is known as a tie line. The intersection of this line with the phase boundaries give the equilibrium compositions of the respective phases..

**TILT BOUNDARY:** See *Grain Boundary*.

**TTT DIAGRAM:** Short for time-temperature-transformation diagram. It represents the time taken to start and complete a transformation as a function of temperature. TTT diagram of steels are particularly important to understand various heat treatments. These diagrams are also known as isothermal transformation (IT) diagrams.

**TWIN BOUNDARY:** A twin boundary is a boundary between two crystals such that atomic positions in one is mirror image of those of the other. See *Interfaces*.



**TWIST BOUNDARY:** See *Grain Boundary*.

**UNIT CELL:** Any three non coplanar lattice translations define a parallelepiped which is called a unit cell of the lattice or the associated crystal. The whole lattice can be generated by parallel repetition of the unit cells. Thus in effect a single unit cell is capable of describing the entire lattice. A unit cell of a lattice is not unique, a lattice can have infinitely many different unit cells.

One can count the effective number of lattice points belonging to a unit cell by considering the sharing of a given lattice point by adjacent cells. The effective number of lattice points belonging to a unit cell is always an integer. If the effective number of lattice points belonging to a cell is one then it is a primitive unit cell, otherwise it is a nonprimitive unit cell. See *Crystal Coordinate System* for another definition of primitive and non primitive unit cells.

**VACANCY:** A site in crystal which ordinarily should have been occupied by an atom but is vacant at the moment is called a vacancy. There is always a number of vacancies in thermodynamic equilibrium at all temperatures above absolute zero. This equilibrium number of vacancies is given by

$$\frac{n}{N} = \exp\left(-\frac{\Delta H_f}{RT}\right)$$

where  $n$  is the number of vacancies,  $N$  the total number of lattice sites,  $\Delta H_f$  the enthalpy of formation of vacancies,  $R$  the gas constant and  $T$  the absolute temperature.

**VULCANIZATION:** The process of cross-linking the polymer chains of rubber through bonding with sulfur. It is done by heating natural rubber with requisite amount of sulfur.

**WORK HARDENING:** A synonym of strain hardening.

**WEISS ZONE LAW:** If the direction  $[u \ v \ w]$  lies (or is parallel to) the plane  $(h \ k \ l)$  then

$$hu + kv + lw = 0.$$

This is true for all crystal systems.

**YIELD STRESS:** The stress at which plastic deformation begins in a uniaxial tensile loading. For single crystals yield stress is anisotropic, *i.e.*, depends upon the crystallographic direction in which the stress is applied, see *Resolved Shear Stress*.

**YOUNG'S MODULUS:** The ratio of stress to strain in the elastic region of a uniaxially loaded sample is called its Young's modulus. Young's modulus is anisotropic for single crystals.

**ZONE REFINING:** A technique for producing ultrapure silicon for electronic application. A molten zone is repeatedly passes through an otherwise solid rod of Si concentrating the impurities to one end of the rod leaving the other end very pure.

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