PH19141 - PHYSICS OF MATERIALS LTPC

3 0 2 4

Common to I sem. B.E. - Aero, Auto, Civil, Mech& MCT

OBJECTIVES

- To enhance the fundamental knowledge in Physics and its applications relevant to mechanical engineering streams.
- To familiarize students in various experimental setups and instruments that are used to study / determine the various properties of materials.

UNIT I - MECHANICS & PROPERTIES OF MATTER 9

Basic definitions - Newton's laws – forces -solving Newton's equations - constraints and friction - cylindrical and spherical coordinates - potential energy function - conservative and non-conservative forces - central forces - conservation of angular momentum - non-inertial frames of reference - rotating coordinate system - centripetal and coriolis accelerations – Elasticity - stress-strain diagram - bending of beams - cantilever depression - Young's modulus determination - I-shape girders.

UNIT II - CRYSTAL PHYSICS 9

Basis – lattices - symmetry operations and crystal systems -Bravaislattics - atomic radius and packing fraction - SC, BCC, FCC, HCP lattices - Miller indices - diffraction by crystals - reciprocal lattice - interpreting diffraction patterns - crystal growth techniques-Czochralski and Bridgmann, crystal defects.

UNIT III - PHYSICS OF MATERIALS 9

Solid solutions - Hume-Rothery's rules –Gibb's phase rule - binary phase diagrams -isomporhpus systems - tie-line and lever rule - eutectic, eutectoid, peritectic, peritectoid, monotectic and syntectic systems - formation of microstructures - homogeneous and non-homogenous cooling – nucleation - iron-carbon phase diagram - eutectoid steel - hypo and hypereutectoid steel – diffusion - Fick's laws – T-T-T diagrams.

UNIT IV - ENGINEERING MATERIALS & TESTING 9

Metallic glasses – preparation and properties - Ceramics – types, manufacturing methods and properties - Composites – types and properties - Shape memory alloys – properties and applications - Nano-materials – top down and bottom up approaches – properties - Tensile strength – Hardness – Fatigue - Impact strength – Creep - Fracture – types of fracture.

UNIT V - QUANTUM PHYSICS 9

Blackbody problem -Planck's radiation law - duality of light -De Broglie hypothesis - properties of matter waves - wave packets –Schrodinger's equations (time dependent and time independent) - Born interpretation (physical significance of wave function) - probability current - operator formalism (qualitative) - expectation values - uncertainty principle - particle in a box -eigen function and eigen values -Dirac notation (qualitative).

TEXT BOOKS:

1. Bhattacharya, D.K. & Poonam, T. *"Engineering Physics"*. Oxford University Press, 2018.
2. Gaur, R.K. & Gupta, S.L. *"Engineering Physics"*.DhanpatRai Publishers, 2018.
3. Raghavan, V. *"Physical Metallurgy: Principles and Practice"*. PHI Learning, 2019.

REFERENCES
1. Balasubramaniam, R. *“Callister's Materials Science and Engineering”*. Wiley India Pvt. Ltd., 2017.
2. Raghavan, V. *“Materials Science and Engineering : A First course”*. PHI Learning, 2019.
3. Resnick, R., Halliday, D., & Walker, J. *“Principles of Physics*”, Wiley India Pvt., 2018.

LIST OF EXPERIMENTS: PHYSICS LABORATORY (Any 10 experiments) 30

1. Determination of Laser characteristics (wavelength and angular spread).
2. Determination of Young’s modulus by non-uniform bending method
3. Determination of thermal conductivity of a bad conductor – Lee’s Disc method.
4. Determination of velocity of sound and compressibility of liquid – Ultrasonic interferometer
5. Coupled oscillators - Two compound pendulums;
6. Experiment on moment of inertia measurement- Torsional pendulum by resonance,
7. LC circuit, LCR circuit and Resonance phenomena in LCR circuits;
8. Experiments on electromagnetic induction – BH-Curve experiment
9. Determination of thickness of a thin wire – Air wedge method
10. Determination of solar cell characteristics.
11. Measurement of hysteresis loss:B -H curve.
12. Determination of creep characteristics of a metallic wire.

TOTAL PERIODS 75

OUTCOMES:
On completion of the course students will be able to

- Understand foundational mechanics and elastic nature of materials and determine the elastic moduli of materials.
- Apply the basic knowledge of crystallography in materials preparation and treatments.
- Create binary phase diagrams and TTT charts and use them to analyse and measure the properties of alloys.
- Understand various engineering materials, test or measure their properties and use them in suitable applications.
- Understand the concepts of quantum theory and the nature of light and determine the characteristics of a given laser source.

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UNIT I – Mechanics and Properties of Matter

Particle: Dimensions of an object are considered to be negligible and small compared to the coordinates describing its motion.

System of particles: An object represented by two or more particles and is dealt with together is called system of particles.

Rigid body: The distance between any two given points on a rigid body is invariant in time regardless of external forces exerted on it.A rigid body is usually considered as a continuous distribution of mass.

Deformable body: Anybody that changes its shape and/or volume while being acted upon by any kind of external force.

A **force** is a push or a pull exerted on one object by another object. The units of force is newton.

Newton's first law: A body continuous a state of rest or uniform motion unless an external force acts on it.

Newton's first law says that if the net force on an object is zero ($\Sigma F=0$), then that object will have zero acceleration. That doesn't necessarily mean the object is at rest, but it means that the velocity is constant.

The property of a body to remain at rest or to remain in motion with constant velocity is called **inertia**. Newton's first law is often called the law of inertia.

The inertia of an object is measured by its mass. Mass can be determined by measuring how difficult an object is to accelerate. The more mass an object has, the harder it is to accelerate.

Newton's second law:Acceleration of an object produced by a net force is directly proportional to the magnitude of the net force, in the same direction as the net force, and inversely proportional to the mass of the object.

Newton's third law: All forces between two objects exist in equal magnitude and opposite direction.

Newton's first law of motion from Newton's second law of motion

Newton's first law states that a body stays at rest if it is at rest and moves with a constant velocity if already moving, until a net force is applied to it. In other words, the state of motion of a body changes only on application of a net non-zero force.Newton's second law states that the net force applied on a body is equal to the rate of change in its momentum. Mathematically,

$$\vec{F} = \frac{d\vec{p}}{dt}$$

Where, F is the net force, and p is the momentum. Now, we can write the same as,

$$\vec{F} = \frac{d\vec{p}}{dt} \Rightarrow \vec{F} = \frac{d(m\vec{v})}{dt} = \frac{md(\vec{v})}{dt}$$

So, if the net force, F is zero, change in the value of v is be zero i.e., a body at rest will be at rest and a body moving with constant velocity will continue with the same velocity, until a net force is applied. This conclusion is similar to the Newton's first law of motion.
Thus, we can derive Newton's first law of motion using Newton's second law of motion.

Newton's third law of motion from Newton's second law of motion
Consider an isolated system of two bodies A & B mutually interacting with each other, provided there is no external force acting on the system.
Let F_{AB}, be the force exerted on body B by body A and F_{BA} be the force exerted by body B on A.Suppose that due to these forces F_{AB} and F_{BA}, dp_1/dt and dp_2/dt be the rate of the change of momentum of these bodies respectively.

Then, $F_{BA} = dp_1/dt$ ---------- (i)
$F_{AB} = dp_2/dt$ ---------- (ii)
Adding equations (i) and (ii), we get,

$F_{BA} + F_{AB} = dp_1/dt + dp_2/dt$
$\Rightarrow F_{BA} + F_{AB} = d(p_1 + p_2)/dt$

If no external force acts on the system, then
$d(p_1 + p_2)/dt = 0$
$\Rightarrow F_{BA} + F_{AB} = 0$
$\Rightarrow F_{BA} = - F_{AB}$ --------- (iii)

the above equation (iii) represents the Newton's third law of motion (i.e., for every action there is equal and opposite reaction).

Constrained Motion: In some cases a particle is forced to move along a curve or surface. This curve or surface is referred to as a constraint, and the resulting motion is called constrained motion. The particle exerts a force on the constraint, and by Newton's third law the constraint exerts a force on the particle. This force is called the reaction force, and is described by giving its components normal to the motion, denoted N, and parallel to the motion, denoted f.

Constrained motion results when an object is forced to move in a restricted way. For example, it may have to move along a curved track, to slide on a table that may accelerate upwards, to stay in contact with an accelerating wedge, etc.

Constraint Forces adjust themselves according to Newton's Second Law so that the acceleration of an object is just the right value for the object to follow the motion required by the particular constrained.

Friction: In the constrained motion of a particle a common force parallel to the motion of the particle is friction, which typically acts in the direction opposite to that of the motion (i.e., it acts in such a way as to slow the motion of the particle). Experimentally, it is found that the magnitude of the frictional force is proportional to the magnitude of the normal force, i.e., $f = \mu N$, where the proportionality constant, μ is referred to as the coefficient of friction. Typically, its value depends on both the material of the particle and the constraint.

When only static friction opposes the motion of two objects, and other forces on the objects increase, the objects will suddenly start to slide (and the law of kinetic friction will apply). This transition occurs when the static friction reaches its maximum value, and experimentally this limiting value of static friction is a constant fraction of the normal force. Just like the coefficient of kinetic friction, the coefficient of static friction is a dimensionless constant that characterizes the nature of the contact between two surfaces. The coefficient of static friction is generally larger than the coefficient of kinetic friction for those surfaces.

A more important difference than their relative size, however, is the difference between the relationships implied by the static friction coefficient versus that implied by the kinetic friction coefficient. In contrast with the coefficient of kinetic friction (which specifies the exact value of the friction force given the normal force) the coefficient of static friction only specifies the limiting value (maximum) of the static friction force.

The mathematical relationship satisfied by the static friction force acting on object A as a result of its contact with object B is:

$$f^{s}_{AB} \leq \mu_s N_{AB}$$

where the inequality indicates that $\mu_s N_{AB}$ is the maximum size that the static friction force between objects A and B can have.

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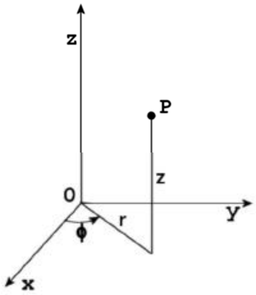
Two coordinate systems that are useful alternatives to Cartesian coordinates in three dimensions. Both cylindrical and spherical coordinates use angles to specify the locations of points, a feature they share with 2-D polar coordinates. spherical coordinates provide a natural way of representing the locations of stars in our local region of the galaxy.

Polar coordinates:The idea behind cylindrical and spherical coordinates is to use angles instead of Cartesian coordinates to specify points in three dimensions. Sometimes, employing angles can make mathematical representations of functions simpler.

Polar coordinatesrepresent points in the coordinate plane, not with the usual Cartesian ordered pair (x, y), but with two different coordinates (r, ϕ)that are functionally related to (x, y). Specifically, for a given point P, r is the absolute distance from the origin to P. The angle ϕ is the angular position of *P*, with angle measured from the positive *x*-axis. Cylindrical and spherical coordinate systems are extensions of 2-D polar coordinates into a 3-D space.

Cylindrical coordinates are most similar to 2-D polar coordinates. Let's consider a point P that has coordinates *(x, y, z)* in a 3-D Cartesian coordinate system. The same point can be represented in cylindrical coordinates *(r, ϕ, z)* where *r* and ϕ are the 2-D polar coordinates of *P*'s image in the *xy* plane ($z = 0$), and *z* is exactly the same as P's Cartesian z-coordinate.



The coordinate transformations to go from Cartesian *x* and *y* coordinates to cylindrical *r* and ϕ coordinates are

$$r = \sqrt{x^2 + y^2}$$

$$\emptyset = \tan^{-1} {}^{y}/_{x}$$

$$Z = Z$$

There are a few features of this transformation to notice. First, the coordinate r under this transformation is always a positive number. ‘r’ is interpreted as the smallest distance from P to the z axis. Also, ϕ, expressed in radians, will always be between -pi and +pi. The z coordinate keeps the same value as you transform from one system to the other. The inverse transformation from (r, theta, z) to (x, y, z) may also be familiar from 2-D polar coordinates as well.

$$X = r\cos\emptyset$$

$$Y = r\,\sin\emptyset$$

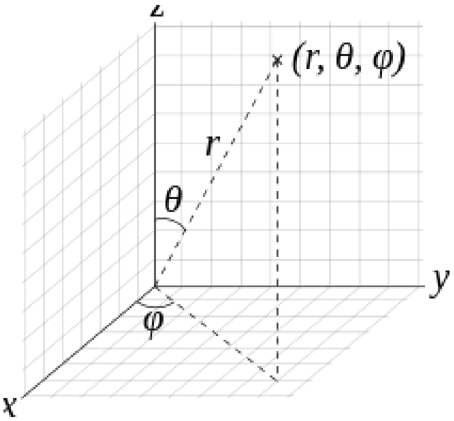
$$Z = Z$$

spherical coordinate system is a coordinate system for three-dimensional space where the position of a point is specified by three numbers: the radial distance of that point from a fixed origin, its polar angle measured from a fixed zenith direction, and the azimuth angle of its orthogonal projection on a reference plane that passes through the origin and is orthogonal to the zenith, measured from a fixed reference direction on that plane.

It can be seen as the three-dimensional version of the polar coordinate system.

The radial distance is also called the radius or radial coordinate. The polar angle may be called colatitude, zenith angle, normal angle, or inclination angle.

The use of symbols and the order of the coordinates differs between sources. In one system frequently encountered in physics (r, θ, φ) gives the radial distance, polar angle, and azimuthal angle, whereas in another system used in many mathematics books (r, θ, φ) gives the radial distance, azimuthal angle, and polar angle.



Potential energy

Let us discuss another form of energy called as potential energy. This is defines for a force field such as the gravitational field or an electric field or elastic field. we define the potential energy of a particle to be the energy that it possesses because of the work done on the particle in moving it from one place to another in a force field. Let us elaborate on this.

Potential energy is closely linked with forces. If the work done by a force on a body that moves from *A* to *B* does not depend on the path between these points (if the work is done by a conservative force), then the work of this force measured from *A* assigns a scalar value to every other point in space and defines a scalar potential field. In this case, the force can be defined as the negative of the vector gradient of the potential field.

If the work for an applied force is independent of the path, then the work done by the force is evaluated at the start and end of the trajectory of the point of application. This means that there is a function $U(\mathbf{x})$, called a "potential," that can be evaluated at the two points $\mathbf{x}_A$ and $\mathbf{x}_B$ to obtain the work over any trajectory between these two points. It is tradition to define this function with a negative sign so that positive work is a reduction in the potential, that is

$$W = \int_C F \, . dX = U(X_A) - U(X_B)$$

where *C* is the trajectory taken from A to B. Because the work done is independent of the path taken, then this expression is true for any trajectory, *C*, from A to B.

The function $U(\mathbf{x})$ is called the potential energy associated with the applied force. Examples of forces that have potential energies are gravity and spring forces.

$$F = \nabla\varphi = \left(\frac{\partial\varphi}{\partial x}, \frac{\partial\varphi}{\partial y}, \frac{\partial\varphi}{\partial z}\right)$$

In this case, work along the curve is given by

$$W = \int_C F \, . dX = \int_C \nabla\varphi \, dx$$

which can be evaluated using the gradient theorem to obtain

$$W = \varphi(X_B) - \varphi(X_A)$$

This shows that when forces are derivable from a scalar field, the work of those forces along a curve *C* is computed by evaluating the scalar field at the start point *A* and the end point *B* of the curve. This means the work integral does not depend on the path between *A* and *B* and is said to be independent of the path.

Potential energy *U*=-φ(**x**) is traditionally defined as the negative of this scalar field so that work by the force field decreases potential energy, that is

$$W = U(X_A) - U(X_B)$$

In this case, the application of the del operator to the work function yields,

$$\nabla W = -\nabla \mathrm{U} = -\left(\frac{\partial U}{\partial X}, \frac{\partial U}{\partial Y}, \frac{\partial U}{\partial Z}\right) = F$$

and the force **F** is said to be "derivable from a potential.This also necessarily implies that **F** must be a conservative vector field. The potential *U* defines a force **F** at every point **x** in space, so the set of forces is called a force field.

Conservative force

It is a force with the property that the total work done in moving a particle between two points is independent of the taken path. Equivalently, if a particle travels in a closed loop, the net work done (the sum of the force acting along the path multiplied by the displacement) by a conservative force is zero.

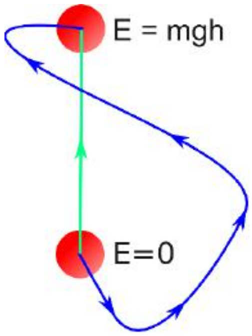
A conservative force is dependent only on the position of the object. If a force is conservative, it is possible to assign a numerical value for the potential at any point. When an object moves from one location to another, the force changes the potential energy of the object by an amount that does not depend on the path taken, contributing to the mechanical energy and the overall conservation of energy. If the force is not conservative, then defining a scalar potential is not possible, because taking different paths would lead to conflicting potential differences between the start and end points.

Gravitational force is an example of a conservative force, while frictional force is an example of a non-conservative force. Other examples of conservative forces are force in elastic spring, electrostatic force between two electric charges, and magnetic force between two magnetic poles. The last two forces are called central forces as they act along the line joining the centres of two charged/magnetized bodies. Thus, all central forces are conservative forces.

Path independence

A direct consequence of the closed path test is that the work done by a conservative force on a particle moving between any two points does not depend on the path taken by the particle.

This is illustrated in the figure to the right: The work done by the gravitational force on an object depends only on its change in height because the gravitational force is conservative. The work done by a conservative force is equal to the negative of change in potential energy during that process. For a proof, imagine two paths 1 and 2, both going from point A to point B. The variation of energy for the particle, taking path 1 from A to B and then path 2 backwards from B to A, is 0; thus, the work is the same in path 1 and 2, i.e., the work is independent of the path followed, as long as it goes from A to B.



For example, if a child slides up a frictionless slide, the work done by the gravitational force on the child from the down of the slide to the up will be the same no matter what the shape of the slide; it can be straight or it can be a spiral or conical. The amount of work done only depends on the vertical displacement of the child.

Mathematical Description:

A force field F, defined everywhere in space (or within a simply-connected volume of space),is called a conservative force or conservative vector field if it meet the following condition. There is zero net work (*W*) done by the force when moving a particle through a trajectory that starts and ends in the same place

$$W = \oint \vec{F} . \overrightarrow{dr} = \vec{0}$$

Non-conservative force

The work done in going from A to B depends on the path taken. Examples of non-conservative forces are friction and non-elastic material stress. Despite conservation of total energy, non-conservative forces can arise in classical physics due to neglected degrees of freedom or from time-dependent potentials. For instance, friction may be treated without violating conservation of energy by considering the motion of individual molecules; however that means every molecule's motion must be considered rather than handling it through statistical methods. For macroscopic systems the non-conservative approximation is far easier to deal with than millions of degrees of freedom.

Central forces

A central force is one which at every point of its field, is directed either towards or away from some fixed point in the field. It can be written as

$$\mathrm{F} = \hat{r} f(r)$$

Where$\hat{r}$ is the unit vector in the direction of position vector r with the field vector r with the fixed point as orgin.

As a consequence of being conservative, these specific central force fields are irrotational, that is, its curl is zero, except at the origin.

$$\nabla \times \mathrm{F}(r) = 0$$

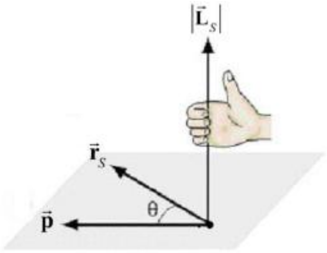
Gravitational force and Coulomb force are two familiar examples
with F(r) being proportional to $1/r^2$ only.

Angular momentum

Angular momentum (rotational momentum) is the rotational equivalent of linear momentum. It is an important quantity in physics because it is a conserved quantity—the total angular momentum of a closed system remains constant.

In three dimensions, the angular momentum for a point particle is a pseudovector r × p, the cross product of the particle's position vector r (relative to some origin) and its momentum vector; the latter is p = *m*v in Newtonian mechanics. This definition can be applied to each point in continua like solids or fluids, or physical fields. Unlike momentum, angular momentum does depend on where the origin is chosen, since the particle's position is measured from it.

Angular momentum is additive; the total angular momentum of any composite system is the (pseudo) vector sum of the angular momenta of its constituent parts. For a continuous rigid body, the total angular momentum is the volume integral of angular momentum density.



By definition, for a single particle moving with linear momentum P at a distance from the orginthe angular momentum L is given as

$$L = r \times P$$

From its definition, it is immediately evident that angular momentum is an orgin-dependent quantity. If we calculate it with respect to some other point, it will come out to be different. The rate of change of angular momentum of a single particle is

$$\frac{dL}{dt} = \frac{d(r \times P)}{dt}$$

$$= \frac{dr}{dt} \times P + r \times \frac{dp}{dt}$$

$$\frac{dL}{dt} = r \times F = \tau$$

The rate of change of angular momentum is equal to the torque applied on the particle.

Conservation of angular momentum

A rotational analogy of Newton's third law of motion might be written, "In a closed system, no torque can be exerted on any matter without the exertion on some other matter of an equal and opposite torque. Hence, angular momentum can be exchanged between objects in a closed system, but total angular momentum before and after an exchange remains constant.

The conservation of angular momentum is used in analysing central force motion. If the net force on some body is directed always toward some point, the centre, then there is no torque on the body with respect to the centre, as all of the force is directed along the radius vector, and none is perpendicular to the radius. Mathematically, torque because in this case and are parallel vectors.

Therefore, the rate of change of angular momentum of a particle system is equal to the total external torque applied to it. If τ is equal to zero then

$$\frac{dL}{dt} = 0$$

L is constant.

An example of conservation of angular momentum is seen in an ice skater executing a spin. The net torque on her is very close to zero, because there is relatively little friction between her skates and the ice, and the friction is exerted very close to the pivot point.

An ice skater is spinning on the tip of her skate with her arms extended. Her angular momentum is conserved because the net torque on her is negligibly small. In the next image, her rate of spin increases greatly when she pulls in her arms, decreasing her moment of inertia. The work she does to pull in her arms results in an increase in rotational kinetic energy.

Inertial frame of reference

A coordinate system in which Newton's first law of motion holds good, is known as an inertial frame of reference. In an inertial frame of reference a body continuous in its state of rest or of uniform motion in a straight line as long as no external force acts on it. All the Newton's law of motion hold good in an inertial frame .All frames of reference moving with a constant velocity with respect to an inertial frame are also inertial frames of reference. It can be called an unaccelerated frame of reference.

An inertial frame of reference may also be called an inertial reference frame, inertial frame, Galilean reference frame, or inertial space. All inertial frames are in a state of constant, rectilinear motion with respect to one another; an accelerometer moving with any of them would detect zero acceleration. Measurements in one inertial frame can be converted to measurements in another by a simple transformation (the Galilean transformation in Newtonian physics and the Lorentz transformation in special relativity). In general relativity, in any region small enough for the curvature of spacetime and tidal forcesto be negligible, one can find a set of inertial frames that approximately describe that region.

Non-inertial frame of reference

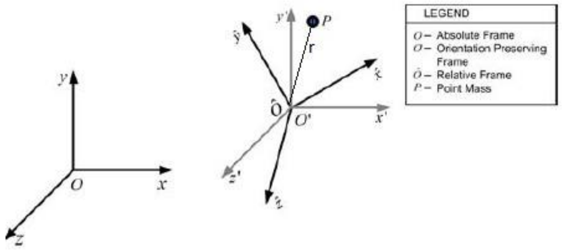
The basic laws of physics are not changed in form in inertial frames of reference. But when a frame of reference is accelerated relative to an inertial frame the form of basic physical laws such as Newton's second law of motion becomes completely different. Such frame of references are called non-inertial frame of reference. A non-inertial frame is either a frame having uniform linear acceleration or a frame which is uniformly rotating.

Earth is not an inertial frame. It is a non-inertial frame. The earth is a rotating sphere as it rotating about its own axis. It has a centripetal acceleration due to rotation. The reference frame attached to the earth is an accelerated frame, so it is a non-inertial.

Rotating coordinate system

A rotating frame of reference is a special case of a non-inertial reference frame that is rotating relative to an inertial reference frame. An everyday example of a rotating reference frame is the surface of the Earth.

Let XYZ represent the cartesian co-ordinate axes of the frame ‘b’ and X^1 Y^1Z^1 those of the frame ‘a’ rotating with angular velocity $\vec{\omega}$ with respect to the frame ‘b’ considered as inertial frame, about an axis passing through the common origin O. The rotating frame of reference ‘a’ is non-inertial frame.



Reference frames used to describe point P

In the inertial frame ‘b’ the position vector of a point P is represented by

$$\overrightarrow{OP} = \vec{r} = x\hat{\imath} + y\hat{\jmath} + z\hat{k}$$

Where x,y,z are the co-ordinates of the point P and $\hat{\imath}, \hat{\jmath}, \hat{k}$ the unit vectors along the X,Y and Z directions respectively in the non-rotating frame ‘b’.

The components of the position vector $\vec{r}$ in the rotating non-inertial frame ‘a’ are represented by

$$\vec{r} = x'\widehat{\imath'} + y'\widehat{\jmath'} + z'\widehat{k'} \qquad \text{(i)}$$

Where x’,y’,z’ are the co-ordinates of the point P and $\hat{\imath}', \widehat{\jmath'}, \widehat{k'}$ the unit vectors along the X’,Y’ and Z’ directions respectively in the non-rotating frame ‘a’.

As the frame ‘a’ is rotating the direction of X^1 Y^1 and Z^1 axes are continuously changing. The directions of unit vectors $\widehat{\imath'}, \widehat{\jmath'}, \widehat{k'}$, are also continuously changing.

Hence, $\widehat{\imath'}, \widehat{\jmath'}, \widehat{k'}$ although constant in magnitude keep on changing direction.

$\frac{d\widehat{\imath'}}{dt}, \frac{d\widehat{\jmath'}}{dt}$ and $\frac{d\widehat{k'}}{dt}$ are not zero.

But unit vectors $\hat{\imath}, \hat{\jmath}$ and $\hat{k}$ in the inertial ‘b’ are constant in magnitude as well as in direction.

$\frac{d\hat{\imath}}{dt}, \frac{d\hat{\jmath}}{dt}$ and $\frac{d\hat{k}}{dt}$ are zero.

Differentiating equation (i) with respect to t,

$$\left(\frac{d\vec{r}}{dt}\right) = \frac{dx'}{dt}\widehat{\imath'} + \frac{dy'}{dt}\widehat{\jmath'} + \frac{dz'}{dt}\widehat{k'} + \hat{x}\frac{d\widehat{\imath'}}{dt} + \hat{y}\frac{d\widehat{\jmath'}}{dt} + \hat{k}\frac{d\widehat{k'}}{dt} \qquad \text{(ii)}$$

$\frac{dr}{dt} = \vec{v}_b$the velocity of the particle P with respect to the inertial frame ‘b’ (X’Y,Z).

$\frac{dx\prime}{dt}\hat{\imath'}+\frac{dy\prime}{dt}\hat{\jmath'} + \frac{dz\prime}{dt}\hat{k'} = \vec{v}_a$ is the velocity of the particle P with respect to the rotational frame ‘a’.

As the linear velocity of a particle is given by $\frac{dr}{dt} = \vec{\omega} \times \vec{r}$, where $\vec{\omega}$ is the angular velocity.

The equation (ii) can be written as $\left[\frac{d\vec{r}}{dt}\right]_b = \left[\frac{d\vec{r}}{dt}\right]_a + \vec{\omega} \times \left(x'\hat{\imath'} + y'\hat{\jmath'} + z'\hat{k'}\right)$

$$= \left[\frac{d\vec{r}}{dt}\right]_a + \vec{\omega} \times \vec{r}$$

$$\vec{v}_b = \vec{v}_a + \vec{\omega} \times \vec{r} = \vec{v}_a + \vec{v}_o \qquad \text{(iii)}$$

The velocity of the particle in the inertial frame $\vec{v}_b$is equal to the vector sum of its velocity in the rotating frame $\vec{v}_a$ and the linear velocity due to its rotation $\vec{v}_o$ the value of which at any instant depends upon the value of $\vec{r}$ at that instant.

Similarly, applying the operator equation to the velocity vector of $\vec{v}_b$ instead of displacement vector $\vec{r}$

$$\left[\frac{d\vec{v_b}}{dt}\right]_b = \left[\frac{d\vec{v_b}}{dt}\right]_a + \vec{\omega} \times \vec{v}_b$$

Substituting the value of $\vec{v}_b$ from (iii) on the right hand side of the above equation and simplify we will get

$$\vec{a}_b = \vec{a}_a + 2\vec{\omega} \times \vec{v}_a + \vec{\omega} \times (\vec{\omega} \times \vec{r}) + \left[\frac{d\vec{\omega}}{dt} \times \vec{r}\right]_a$$

Where $\vec{a}_a$ is the acceleration in the rotating frame ‘a’ and$\vec{a}_b$ is the acceleration in the stationary frame ‘b’.

The term $2\vec{\omega} \times \vec{v}_a$ is known as Coriolis acceleration after the name of its discoverer. The term appears only when the particle moves in the rotating frame.

The term $\vec{\omega} \times (\vec{\omega} \times \vec{r})$ is the centripetal acceleration. The last term $\frac{d\vec{\omega}}{dt} \times \vec{r}$ is the acceleration due to change in $\vec{\omega}$. This is zero when the angular velocity $\vec{\omega}$ of the rotating frame is a constant.

Coriolis force is defined as the fictitious force which acts on a particle when it is in motion relative to a rotating frame of reference.

Elasticity

When we apply a force on a solid object, it may deform (Change in shape and/or size). The property by which the body regains its original shape and size, on removal of the deforming force is called Elasticity.

Perfect Elastic bodies

If a body resists deformation and recovers its original size or volume completely and immediately on the removal of the deforming forces it is called perfectly elastic body.

If it completely retains its altered shape and size, it is said to be**perfectly plastic.**

In general bodies are in between these two extreme limits. There is no perfectly elastic (or) perfectly plastic body.

Stress and strain

When a body is subjected to a force or a system of forces it undergoes a change in size or shape or both when the force is applied. The applied forces stored as a potential energy in the body when the deforming force is removed it restore its original shape and size.

The change per unit length is called **strain** or generally expressed as change in dimension to original dimension

$$\text{Strain}=\frac{\text{change in dimension}}{\text{original dimension}}$$

Strain has no units.

There are three types of strain; they are explained in detail as follows:

1. **Longitudinal or Tensile Strain**
   The change in length per unit original length without any change in shape is called as longitudinal strain.
2. **Shear or Shearing Strain**
   When tangential forces act on a body, it undergoes a change in shape. The angular deformation produced is called shearing strain or shear.
3. **Volumetric Strain**
   It is defined as the change in volume per unit original volume, without any change in shape.

Hooke's Law

According to this law the stress is proportional to strain producing it within elastic limit

$$\text{Stress } \alpha \text{ strain}$$

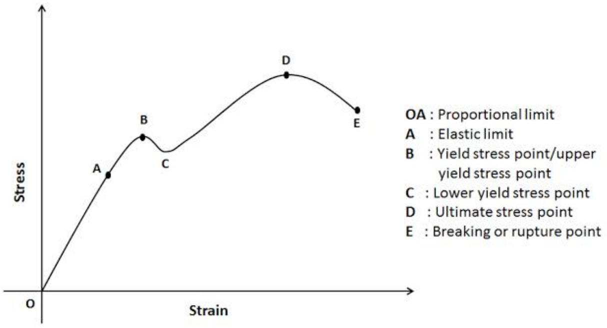
$$\text{Or } \frac{Stress}{Strain} = \text{ a constant} = E$$

The constant E is called the co efficient of Elasticity or modulus of Elasticity. The value of this constant depends upon the nature of the material

It has the same unit of stress that is Nm^{-2} Or Pascal

Stress –Strain diagram

We can plot a graph between stress and strain for a ductile material such as copper or low carbon steel until it breaks. There are number of important points to be observed in such graph.



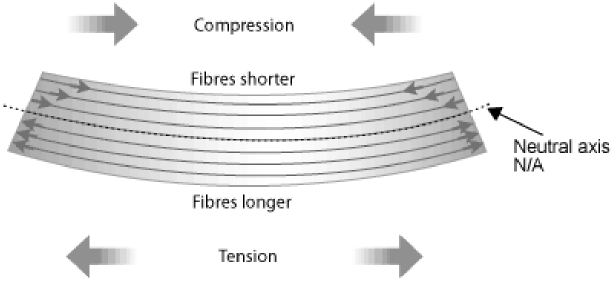
Stress-Strain curve for ductile materials

It is clear from this graph that Hooke's law holds good only for the straight line

1. Within (OA) the wire regain its original length on the removal of the applied load, the wire within OA obey Hooke's law
2. Beyond A up to B even for the smallest increase in stress larger strain is produced in the body. B is called Elastic Limit
3. If the wire is loaded beyond the elastic limit elongation is permanent and a stage is reached where the elongation is continues without further loading up to C and this point is called Yield point
4. Beyond elastic limit, a permanent set (OD) is produced in the wire
5. Beyond the yield point, even for very small increase in load, the extension increases rapidly and the wire becomes thinner. Beyond D, called breaking strength, the wire may break at any stage.

Bending Moment

A beam is defined as rod of uniform cross-section whose length is much greater as compared to its other dimensions, so that shearing stresses over any section of it are negligibly small. They are usually set in horizontal position and are designed to support heavy loads. They are used in building to support roofs and in bridges to support the load of vehicles passing over them.

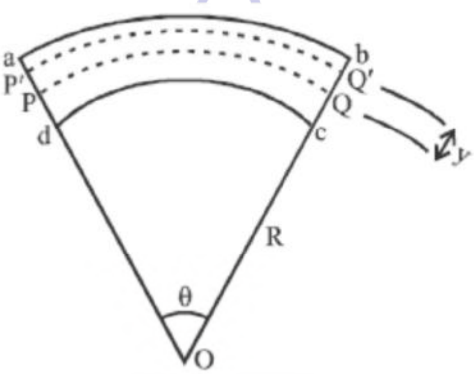


A bending of a beam

Let us consider a beam of uniform rectangular cross section as shown in the Fig.1.12. A beam may be assumed to consist of a number of parallel longitudinal metallic fibers placed one over the other and are called as filaments. Under the bent condition, the convex side of the beam is extended while those on the concave side are compressed. In between these filaments, this is neither lengthened nor shortened, but remains constant in length. This filament is called **neutral filament** and the axis of the beam lying on the neutral filament is called the **neutral axis**. Further the deformation of any filament can be measured with reference to neutral axis.

Derivation of bending moment of beam

Let us consider the section abcd in Figure represents a small longitudinal bent beam. Let PQ represent a filament at the neutral surface and P'Q' another filament at distance y from PQ. In a bent beam, PQ and P'Q' are arcs of a circle having their centre at O and of radii R and R + y respectively. If θ is the angle for POQ,



Bending moment of a beam

we have
$PQ = R\,\theta$
and $P'Q' = (R+y)\,\theta$

Change in length produced in the filament PQ due to bending $= P'Q' - PQ$

$$= (R + y)\theta - R\theta$$

$$= R\theta + y\theta - R\theta$$

$$= y\theta$$

The extensional strain on the filament $= \dfrac{\text{change in the length}}{\text{original length}}$

$$= \frac{Y\theta}{R\theta}$$

$$= \frac{Y}{R}$$

Since the beam is not subjected to either shearing or bulk strain the extensional or compressional strains on the filaments are due to forces acting along the length of the filaments.

If Y is the Young's modulus of the material of the beam the longitudinal stress on the filament P' Q'.

$$= Y \times \text{Strain}$$

$$= Y \times \frac{y}{R}$$

Let a be the area of cross section of the filament.
The longitudinal force on the filament is stress × area

$$\text{Longitudinal force} \quad = \frac{y}{R} \times a$$

$$= \frac{Yy}{R} a$$

The moment of the longitudinal force about the neutral axis = Force × distance

$$= \frac{Yy}{R} a \times y$$

$$= \frac{Y}{R} a\, y^2$$

As the moment of the forces acting on both the upper and lower halves of the section are in the same direction, the total moment of forces acting on the filaments due to straining

$$= \sum \frac{Y}{R} a\, y^2$$

$$= \frac{Y}{R} \sum ay^2$$

Here, the quantity $\sum ay^2$ is the geometrical moment of inertia and is equal to AK^2, A being the total area of the section and K being the radius of gyration of the beam. The quantity $\sum$ ay2 is represented as Ig where Ig is the geometrical moment of inertia of the bar. The total moment of forces acting on all the filaments is called bending moment.

$$\text{Bending moment} = \frac{YAK^2}{R}$$

$$\text{Bending moment of the beam} = \frac{Y}{R} I_g$$

Case (i)For rectangular cross section

If b is the breadth and d is the thickness of the beam, then

$$\text{Area } A = bd \text{ and } K^2 = \frac{d^2}{12}$$

$$Ig = AK^2 = \frac{bd.d^2}{12} = \frac{bd^3}{12}$$

Substituting the value of Ig in the bending moment of a beam equation

$$\text{Bending moment for a rectangular cross section} = \frac{Ybd^3}{12R}$$

Case (ii) For a circular cross section if r is the radius, then area $A = \pi r^2$

And $K^2 = \frac{r^2}{4}$

$$Ig = AK^2 = \frac{\pi r^2 \times r^2}{4}$$

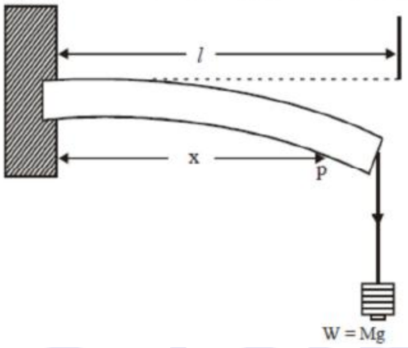
$$Ig = \frac{\pi r^4}{4}$$

Substituting value of Ig in the bending of a beam equation, then the equation becomes

$$\text{Bending moment for a circular cross section} = \frac{\pi Y r^4}{4R}$$

Cantilever

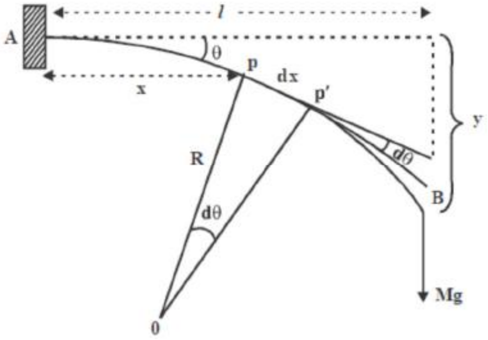
A beam clamped horizontally at one end and loaded with a weight at the free end is called a **cantilever**.



Cantilever

Consider a section at P at a distance x from the fixed end. Neglecting the weight of the part between P and the free end, the moment of the external couple = Mg(l - x).

The bending moment of the section at P = $\frac{YAK^2}{R}$, where R is the radius of curvature of the neutral axis at P



Depression at the free end of cantilever

At equilibrium, $Mg(l - x) = \frac{YAK^2}{R}$

$$R = \frac{YAK^2}{Mg(l-x)}$$

From this expression we find that as x increases, R also increases, the maximum and minimum values being at the free and fixed ends respectively. Since the radius of curvature of the neutral axis (R) varies from point to point of the cantilever (x), the bending is said to be non-uniform.

Let P' be another point on the bent cantilever at a small distance dx from P. Since P and P'are very near we can assume that the radius of curvature R is practically the same and O is its centre of curvature.

Let the angle between the tangents at P and P'be dθ.

Then angle POP' = dθ

$$dx = Rd\theta$$

$$R = \frac{dx}{d\theta}$$

substituting the equation (2) in (1)

$$Mg(l-x) = YAK^2\frac{d\theta}{dx}$$

$$d\theta = \frac{Mg(l-x)dx}{YAK^2}$$

If θ is the angle between the tangents at A and B, we have

$$\theta = \int_0^l \frac{Mg(l-x)dx}{YAK^2}$$

$$\theta = \frac{Mgl}{YAK^2}\int_0^l dx - \frac{Mg}{YAK^2}\int_0^l xdx$$

Deflection of cantilever= $\frac{Mgl^2}{2YAK^2}$

If dy is the depression of B due to the curvature at PP'

$$dy = (l-x)d\theta$$

$$d\theta = \frac{dy}{l-x}$$

Substituting the equ.(5) in (3)

$$dy = \frac{Mg(l-x)^2dx}{YAK^2}$$

The depression y is given by

$$Y = \int dy = \int_0^l \frac{Mg(l-x)^2\,dx}{YAK^2}$$

$$= \frac{Mg}{YAK^2}\int_0^l (l-x)^2\,dx$$

$$= \frac{Mg}{YAK^2}\left[l^2x - \frac{2lx^2}{2} + \frac{x^3}{3}\right]_0^l$$

$$= \frac{Mg}{YAK^2}\left[l^3 - l^3 + \frac{l^3}{3}\right]$$

Depression of cantilever $y = \dfrac{Mgl^3}{3YAK^2}$

Case i For rectangular cross section

If b is the breadth and d is the thickness of the beam then Ig becomes

$$\text{Ig} = \frac{bd^3}{12}$$

Substituting the value of Ig in the above (cantilever) equation

The depression produced at free end for a rectangular cross section

$$y = \frac{Mgl^3}{3Y\dfrac{bd^3}{12}}$$

$$y = \frac{4Mgl^3}{3Ybd^3}$$

Case ii For circular cross section, If r is the radius of the circular cross section, then

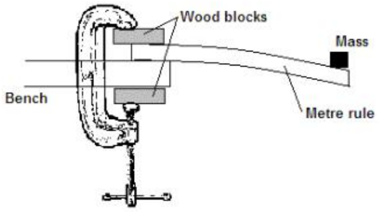
$$Ig = \frac{\pi r^4}{4}$$

Substituting the value of Ig in the above (cantilever) equation

Depression produced $y = \dfrac{Mgl^3}{3Y(\pi r^4/4)}$, $\quad y = \dfrac{4Mgl^3}{3\pi Yr^4}$

Experimental Determination of Young’s Modulus byCantilever

A given beam one end is clamped by using a clamp on the table and free end is allowed to add load using weight hanger is as shown in the Figure. A pin p is fixed at the free end of the beam by using wax. A travelling microscope is place in front of the whole setup for finding the position of the pin. Initially, the beam is brought into elastic mood by loading and unloading it several times. Now, with the weight hanger alone as the load, the travelling microscope is adjusted until its horizontal cross-wire coincides with the tip of the pin. The corresponding vernier scale reading is noted.



Cantilever experiment

Taking the weight hanger as the dead load (W), the microscope is adjusted and the tip of the pin is made to coincide with the vertical cross wire. The reading is noted from the vertical scale of the microscope. Then weights are added (loading) to the weight hanger in steps of 50 gmsupto to a total of 250 gms. In each case, it is ensured that the horizontal cross-wire coincides with the tip of the pin as in Fig. and the corresponding vertical scale readings are noted. The procedure is repeated by removing the weights (unloading) in the same steps of 50 gms each and the microscope readings are taken as before for the corresponding loads.

The mean of loading and unloading readings for each load M is recorded. The breadth b and the thickness t of the beam are measured by vernier caliper and screw gauge respectively. The observed values are substituted in the formula of Young’s modulus to get the young’s modulus of the material of the given beam by cantilever.

S.No	**Load (gm)**	**Microscope Readings (m)**		**Average**	**Depression for a mass of m=50gm**
		Loading	**Unloading**		
1	W			A	a ≈ b
2	W+50			B	b≈c
3	W+100			C	c≈d
4	W+150			D	d≈e
5	W+200			E	e≈f
6	W+250			F	f≈g
7	W+300			G	
				Average y	

$$Young's\ Modulus\ Y = \frac{4Mgl^3}{3ybd^3}$$

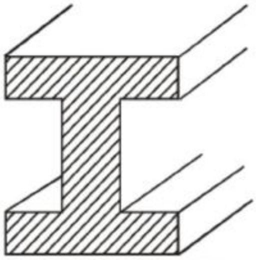
By substituting all the values in the above equation we can calculate the Young's modulus of the given beam.

I-Shaped Girders

In general, a girder bridge is very likely the most commonly built and utilized bridge in the world. Its basic design, in the most simplified form, can be compared to a log ranging from one side to the other across a river or creek

A girder supported at its two ends on the opposite walls of a room, bends under its own weight and, or under the load placed above it. The middle portion gets depressed. The depression (y) at the mid point of a rectangular beam is proportional to $\frac{Mgl^3}{Ybd^3}$. For the depression (y) to be small for a given load (w), the length of the girder (l) should be small and its breadth (b), depth (d) and Young's modulus for its material (Y) must be large.

Due to depression, the upper parts of the beam above neutral surface contract, while those below the neutral surface extended. Hence the stresses have a maximum value at the top and bottom and progressively decrease to zero as we approach the neutral surface from either face.



I shaped girders

Therefore, the upper and lower surfaces of the beam must be stronger than the intervening part. That is why the two surfaces of a girder or iron rails (for railway tracks etc.) are made much broader than the rest of it, thus giving its cross section the shape of the letter I. Hence the girders with I shape are called I-form girders. In this manner, material will be saved, without appreciably impairing its strength. Since the stress experienced at the middle portions of the girders is maximum, removal of the material does not reduce the strength of the girders.

Advantages of I-shaped girders are:

- Economy of material without loss of efficiency.
- Self-loading is minimized.
- Strength of the girders does not fall.

Applications of I shape girders

1. They are used in the construction of bridges over the rivers or roads.
2. They are very much useful in the production of iron rails which are used in railway tracks.
3. They are used in the construction of iron beams to support the bridges for the heavy vehicles.
4. They are used as supporting beams for ceiling in the construction of buildings.

UNIT – II - CRYSTAL PHYSICS

5.1 INTRODUCTION

All materials in this universe can be classified in to five fundamental states (or ‘phase’), namely: i. Solid, ii. Liquid, iii. Gas, iv. Plasma and v. Bose-Einstein Condensate.

All materials, that are in solid state can be further classified in to two types: Crystalline and Amorphous (Non-crystalline).

Crystals are solids whose constituent atoms (or molecules or ions[1]) have a regular and periodic arrangement across all tree spatial dimensions (viz. length, breadth and thickness!)

Amorphous solids will have no such governing arrangement for their constituent atoms.

Many of the properties of solids can be understood based on their microscopic structure, that is, the arrangement of their constituent atoms, and hence the study and knowledge of crystal structures becomes inevitable for a material scientist or an engineer (who uses a variety of materials for his/her applications.)

The study of determining and analysing the crystal structure is known as ***crystallography***.

The regularity and periodicity of crystal arrangement can be studied by understanding the ***basis***, the ***lattice*** and the ***unit cell*** structure of a given crystal.

5.2 BASIS

The particular minimal arrangement of atom(s) which, when repeated along all three dimensions, gives us the actual crystal itself will be called as the ‘basis’ of that crystal.

For example, in many pure metal specimen (say copper or iron), a single atom of that metal will form the basis for its crystal structure.

In a sodium chloride salt sample, a single molecule of sodium chloride acts as the basis for the crystal.

5.3 LATTICES

Lattice is a mathematical concept. For studying the crystal structures, we consider what is known as a ‘space lattice’.

- A lattice is a collection of points - in 3 dimensional space
- Each and every point in a lattice should have the same environment

That is, the arrangement of other points around a given lattice point should be identical for all points in a given lattice.

Only those collection of points which satisfy both the above conditions can be called as a lattice. However, the second condition can only be satisfied if the collection is infinite (for

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[1] Henceforth, any mention of atom will equally apply to molecules and ions, unless specified otherwise.

any finite collection will have different arrangement of points inside its volume and near its edges (boundaries)).

Since crystal specimen are not infinite in size, we need only a portion of an actual lattice to represent the periodicity of the crystal and such a portion is what is called as a space lattice.

Lattices in Different Dimensions

There is only one possible lattice in **1 dimension**.

A collection of points equally spaced along a straight line is the one-dimensional lattice (Fig. 5.1). The position of any point in such a lattice can be mathematically represented as below,

$$\vec{R} = n\vec{a}$$

Where $\vec{a}$ is the primitive vector defining the lattice and n is any integer (both positive and negative).

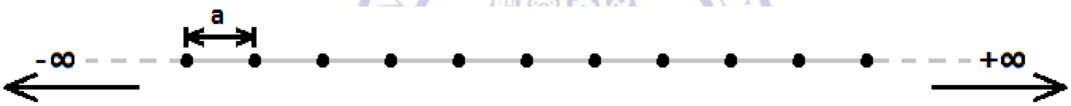


Fig. 5.1 – One dimensional lattice

There are five possible unique lattices in **2 dimensions**. These are the i. Oblique, ii. Rectangular, iii. Centred Rectangular, iv. Square and v. Hexagonal. These are shown below (Fig. 5.2).

The positions of lattice points in a 2-dimensional lattice can be defined using two primitive vectors, as shown below,

$$\vec{R} = n_a\vec{a} + n_b\vec{b}$$

Where n_a and n_b are integers.

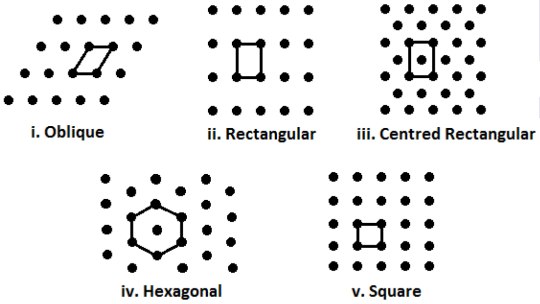

i. Oblique
ii. Rectangular
iii. Centred Rectangular
iv. Hexagonal
v. Square

Fig. 5.2 – Two dimensional lattices

Similarly, there are only fourteen possible unique lattices in **3 dimensions**. These are know as the **Bravais Lattices** (pronounced as *'bra-ve'*, named after the French physicist Auguste Bravais, 1811 – 1863)

We shall discuss these in detail in a later section.

5.4 UNIT CELL

The minimum portion of a crystal lattice that completely defines the symmetry and structure of the entire crystal is known as the unit cell.

Unit cells can be thought of as the building blocks with which the entire crystal is built.

Primitive and Non-primitive Cells

Unit cells that consists of only one lattice point are called as primitive cells and those which contain more than one lattice points are called as non-primitive cells. Primitive cells are also known as simple unit cells (denoted by ‘P’).

Unit cells of seven lattices out of the fourteen Bravais lattices are primitive.

Unit Cell vs Basis

Basis is the entity that is repeated along the lattice points in all three dimensions to get the crystal structure. However, the shape (symmetry) of the structure cannot be identified from the basis. It is the unit cell that gives us that information.

For example, Polonium has simple cubic structure (figure 5.3). The basis for the crystal is a single polonium atom – when this is added to each and every lattice point we get the polonium crystal.

This single atom basis does not tell us the simple cubic structure. It is the unit cell that lets us identify the lattice structure. Thus the minimum portion of the lattice that completely represents the structure of the lattice is the unit cell.

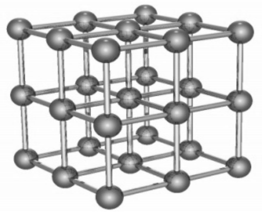


Fig. 5.3 – Polonium unit

Unit Cell Parameters and Crystal Axes

Positions of lattice points in a three dimensional lattice can be represented by using three primitive vectors, as below,

$$\vec{R} = n_a\vec{a} + n_b\vec{b} + n_c\vec{c}$$

Where n_a, n_b, and n_c are integers and $\vec{a}$, $\vec{b}$, and $\vec{c}$ are the primitive vectors of the lattice.

The magnitude of these primitive vectors a, b, and c and the angle between them α, β, and γ respectively are known as the unit cell parameters or lattice parameters.

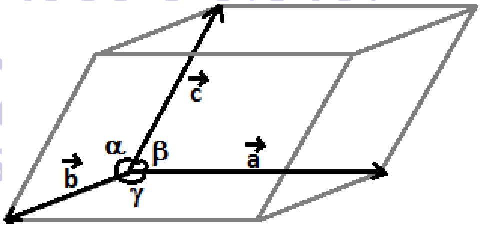


Fig. 5.4 – Unit cell parameters

Single Crystalline and Polycrystalline Materials

Single crystals or *mono-crystalline solids* are those in which the crystal lattice of the entire specimen is continuous and unbroken from edge to edge without any grain boundaries.

Single crystals, due to the lack of grain boundaries and the defects associated with them, have their properties enhanced in most cases and are sought after for many applications.

A ***Polycrstalline material*** is made up of many small single crystals, each known as a *grain* or *crystallites* (the term *domain* is also used to refer to them). The size, shape, and orientation of the constituent grains vary from specimen to specimen, even for the same material, and depends very much on the conditions (like temperature, concentration, etc) during growth.

The region where two adjacent grains meet is known as a ***grain boundary***. Grain boundaries are usually weak spots of a crystal – mechanically, optically and in other such aspects.

5.5 SYMMETRY OPERATIONS

Crystals have an ordered internal arrangement of atoms. This uniform arrangement of atoms in crystal shows symmetry, (i.e.) the atoms are arranged are in a symmetrical fashion on a three dimensional network called as "*lattice*". Crystal faces form as smooth planar boundaries that make up the surface of the crystal. These crystal faces reflect the ordered internal atomic arrangements and thus reflect the symmetry of the crystal lattice too. In order to throw light on the case, let's first imagine a 2-dimensional crystal composed of atoms in an periodic arrangement as shown in Figure 5.5. Since all of the atoms in the crystal lattice are the same, for better understanding of symmetry operations look into the grey colour atom in the first image (Left corner atom at the bottom)

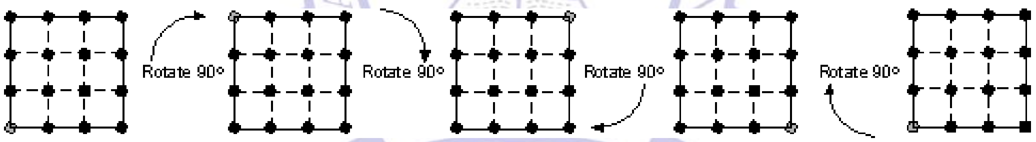


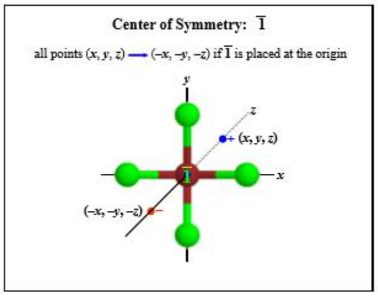
Figure. 5.5 Two-dimensional crystal composed of atoms in a periodic arrangement

If we rotate the crystals by 90^{o} notice that the lattice and crystal look exactly the same as what we started with. Rotate it another 90^{o} and again its the same. Another 90^{o} rotation again results in an identical crystal, and another 90^{o} rotation returns the crystal to its original orientation. Thus, in one 360^{o} rotation, the crystal has repeated itself, or looks identical 4 times. We thus say that this object has 4-fold rotational symmetry.

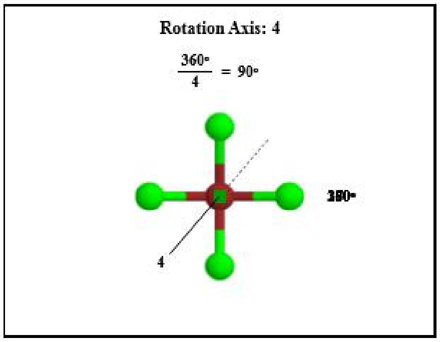
The requirements of a symmetry operation is that when it operates (is used) on an atom with a set of atomic coordinates (x,y,z), an atom of the same type and with identical surroundings is created, but with the coordinates (x',y',z'). These are the symmetry elements which exist:

- ✓ **Identity** – That is (x,y,z) is transferred to itself (x,y,z). This symmetry elements is included, because it is a basic requirement in the definition of a group in group theory, which is the mathematical tool used in symmetry considerations.

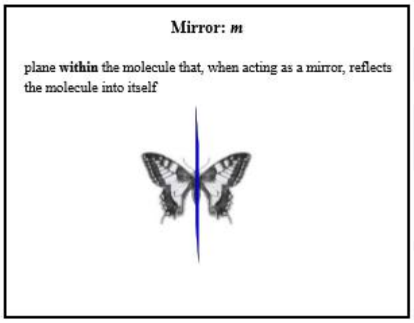
- ✓ **Inversion** – That is (x,y,z) is translated to (-x,-y,-z). If an object has this symmetry element, it is said to be Centro symmetric.



- ✓ **Rotation axis**– A rotation axis is twofold, three fold etc. A ‘n’-fold axis rotate an object 360^o/n.



- ✓ **Mirror Plane (or) Reflection**–Mirror plane which places the object laterally reversed (mirror image) as far behind the mirror plane as it was in front.



Inversion symmetry and mirror planes both transfers a right handed object to a left handedobject, (like a mirror image; this is shown by writing a comma (,) in the circles).

The origin of the symmetry operations and the coordinate system are chosen so as to reveal the highest possible symmetry. Two sets of nomenclature are used to indicate symmetry operations. Schönflies nomenclatures often used in spectroscopy, whereas Hermann-Mauguin nomenclature is used in crystallography. The notation is different, but the operations are of course the same, see Table.

Symmetry Operation	Schönflies Symbol	Hermann-Mauguin

Identity	E (or) I	I
Inversion	I	$\bar{1}$
Rotation axis	C_n(n = fold)	n
Mirror plane	$\sigma_h \sigma_v$	m

σ_h and σ_v are the notation for the horizontal and the vertical mirror plane respectively (definedrelative to the main rotation axis).

There are also combined symmetry operations, which means that two symmetry operations are performed right after each other and thus the “intermediate state” is not considered.Rotation-inversion axes are used in crystallography [rotation-inversion axes are denoted as ‘n’, often expressed as$\bar{n}$], i.e. a n-fold rotation is done followed by an inversion. In the17Schönflies notation rotation-inversion axes are denoted S_n.

5.6 CRYSTAL SYSTEMS AND BRAVAIS LATTICE

As mentioned already, there are only 14 possible unique lattice arrangements in 3-dimensional space. Any other arrangement of points, to form a lattice, will be one of these 14 lattices considered from a different axes set or a linear combination of these.

These 14 are known as the Bravais lattice. The 14 Bravais lattices are grouped in to 7 crystal systems based on their unit cell’s shape and symmetry axes.

The 7 Crystal systems and the 14 Bravais lattices are tabulate below:

Crystal System	**Bravais Lattices**
Cubic	Simple cubic, Body-centered cubic, Face-centered cubic
Tetragonal	Simple tetragonal, Body-centered tetragonal
Orthorhombic	Simple Orthorhombic, Body-centered Orthorhombic, Face-centered Orthorhombic, Base-centered Orthorhombic
Rhombohedral / Trigonal	Simple Rhombohedral/ Trigonal
Hexagonal	Hexagonal close packed
Monoclinic	Simple Monoclinic, Base-centered Monoclinic
Triclinic	Simple Triclinic

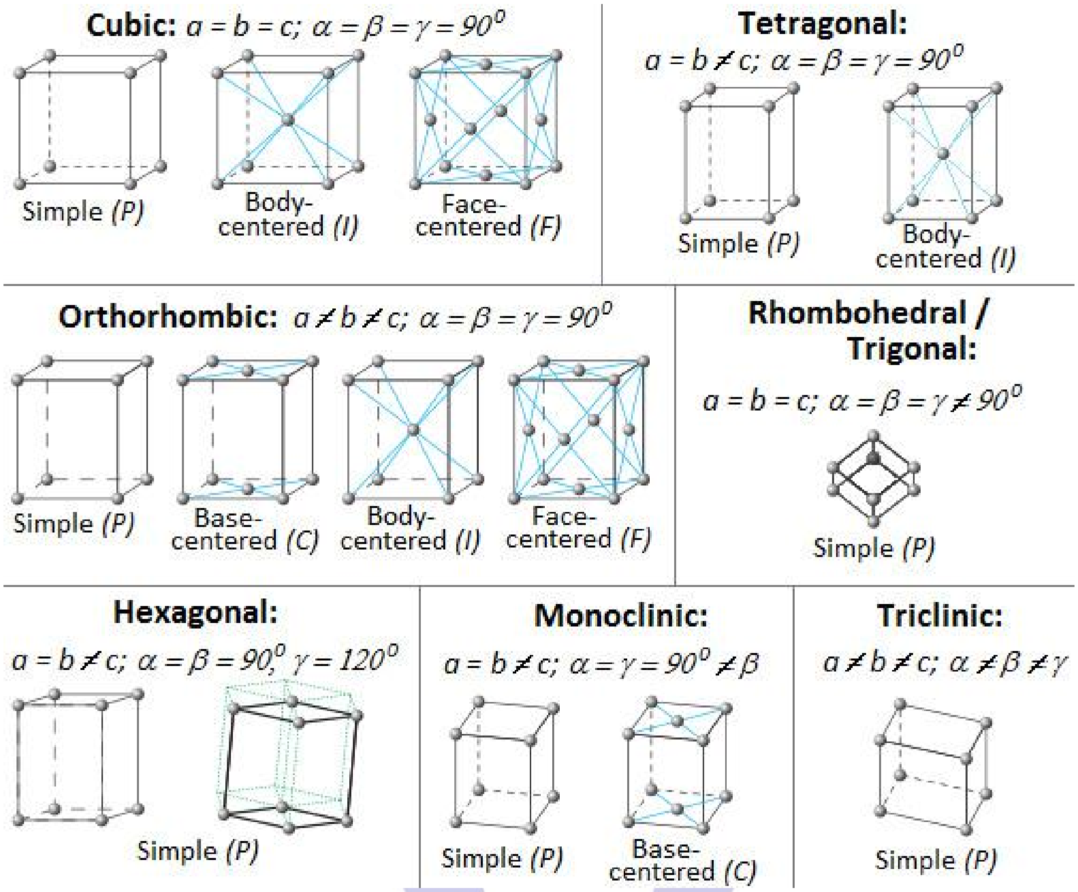


Fig. 5.6 – 14 Bravais Lattices (3D lattices)

5.7 COORDINATION NUMBER

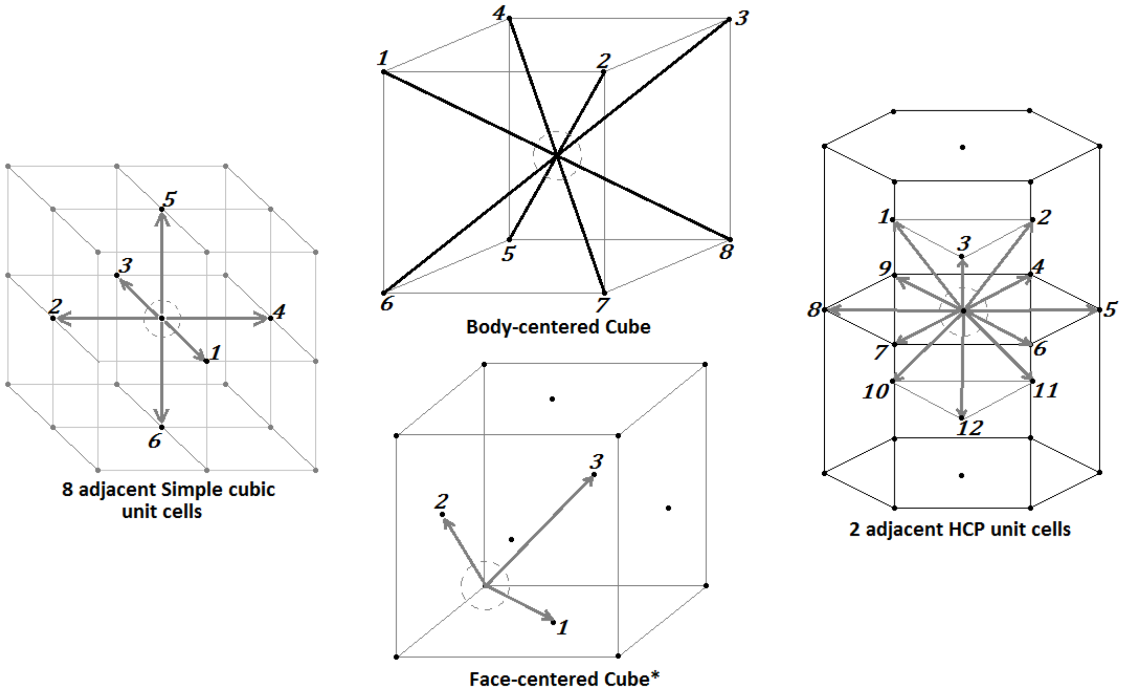
Coordination number refers to the number of nearest lattice points for a given lattice point.

This number corresponds to the interaction between adjacent atoms and can give us certain properties of the material or crystal.

Coordination number for the simple cubic lattice is 6 and that for the Body-centered cubic lattice is 8.

Coordination numbers for the Face-centered cubic lattice and Hexagonal close-packed lattice are both 12.

These are illustrated in the below diagrams:



8 adjacent Simple cubic unit cells

Body-centered Cube

Face-centered Cube*

2 adjacent HCP unit cells

Fig. 5.7 – Coordination number of crystal systems

*In FCC a corner atom has 3 nearest face-centered atoms in one unit cell, hence it will have 12 nearest neighboring atoms in all 8 unit cells of which it belongs.

Note: Coordination number is the same for all lattice points in a lattice (A lattice, by definition, is a collection of points which have the same environment of points, hence the above condition!) Any point can be considered to calculate the coordination number of a lattice. For example, in a BCC lattice the coordination number for a body-centered atom is 8 (being surrounded by eight corner atoms) and the coordination number for a corner atom is also 8 (being surrounded by eight body-centered atoms from the eight adjacent unit cells to which it belongs).

5.8 EFFECTIVE NUMBER (N)

The actual number of atoms (lattice points) in an unit cell is known as **effective number(N).**

Effective Number of a Simple Cubic Lattice

Consider a simple cubic lattice with one atom at every lattice point (i.e. Basis = 1 atom). The unit cell will appear to be made of 8 atoms. However, each of these 8 atoms belongs to 8 adjacent unit cells simultaneously.

Hence the contribution of a single atom for a given unit cell is only 1/8th and thus the effective number of atoms (or lattice points) in that unit cell is given as,

$$N = 8 \text{ corner atoms} \times \frac{1}{8}$$

$N = 1 \text{ atom}$

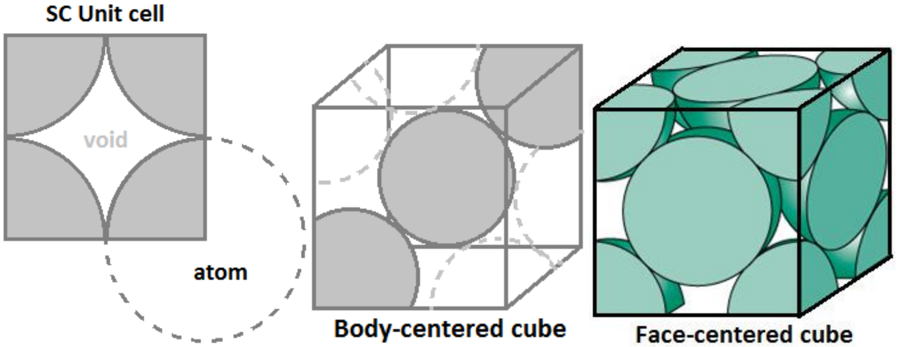


Fig. 5.8 – Effective number of Crystal systems

Effective Number of a Body-centered Cubic Lattice

The body-centered cubic lattice has 1 body-centered atom which is completely inside the BCC unit cell and eight corner atoms that contribute 1/8th to the unit cell.

Hence the effective number of a body-centered cubic lattice is given as,

$$N = (1\text{body-centered atom} \times 1) + \left(8 \text{ corner atoms} \times \frac{1}{8}\right)$$

$$N = 1 + 1 = 2 \text{ atoms}$$

Effective Number of a Face-centered Cubic Lattice

The face-centered cubic lattice has 6 face-centered atoms which belong to two adjacent unit cells thereby contributing ½ to each of the unit cell they belong to. It also has 8 corner atoms which belong to eight adjacent unit cells and contribute 1/8th to the unit cell.

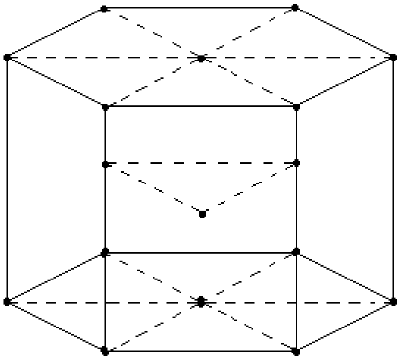
Hence the effective number of a face-centered cubic lattice is given as,

$$N = \left(6 \text{ face-centered atoms} \times \frac{1}{2}\right) + \left(8 \text{ corner atoms} \times \frac{1}{8}\right)$$

$$N = 3 + 1 = 4 \text{ atoms}$$

Effective Number of a Hexagonal Close-packed Lattice

A hexagonal close-packed lattice is made up of alternating hexagonal layers, with the lattice point of any layer being aligned above (or below) the centroid of the triangle made by the atoms in the layer below (or above) it.



HCP unit cell

Thus a HCP unit cell consists of three layers: hexagonal (top), triangular (middle), and hexagonal (bottom).

The top and bottom hexagonal layers consist of 7 atoms each: 1 centre atom belonging 1/2 to the unit cell and 6 corner atoms belonging 1/3 to the unit cell.

The middle triangular layer contains 3 atoms that completely belong to the given unit cell.

Hence the effective number of a hexagonal close-packed lattice is given as,

$$N = \left(2 \text{ center atoms} \times \frac{1}{2}\right) + \left(6 \text{ corner atoms} \times \frac{1}{3}\right) + (3 \text{ middle atoms} \times 1\,)$$

$$N = 1 + 2 + 3 = 6 \text{ atoms}$$

5.9 ATOMIC PACKING FRACTION (APF)

Atomic packing fraction is the ratio of the volume occupied by the atoms in a unit cell to the total volume of the unit cell.

$$APF = \frac{No.\,of\ atoms \times Volume\ of\ each\ atom}{Volume\ of\ the\ unit\ cell} = \frac{N \times V_{atom}}{V_{unit\ cell}}$$

Note: In calculating the atomic packing fraction each atom (or basis) is assumed to be a sphere of radius ‘*r*’, where ‘*r*’ is half the distance between two adjacent lattice points.

Packing Fraction of a Simple Cubic Unit Cell

In a simple cubic lattice, the atomic radius is twice the lattice constant (a), since adjacent atoms ‘*touch’* each other along the unit cell edges (see figure).

Thus the atomic radius in a SC lattice is given as,

$$r = \frac{a}{2}$$

Hence the atomic packing fraction can be calculated as below:

$$APF = \frac{N \times V_{atom}}{V_{unit\,cell}} = \frac{1 \times \left(\frac{4}{3}\pi r^3\right)}{a^3}$$

Using the relation between atomic radius and unit cell dimension (***a-r relation***), *r = a/2*, we get,

$$APF = \frac{\left(\frac{4}{3}\pi \left(\frac{a}{2}\right)^3\right)}{a^3} = \frac{\pi}{6}$$

Or,

$$APF = \frac{\pi}{6} \cong 0.52$$

Thus the packing fraction of a simple cubic lattice is 0.52 or 52%. This means that only 52% of the volume is occupied by atoms and the remaining 48% is empty – this empty space inside a crystal lattice is known as ***void***.

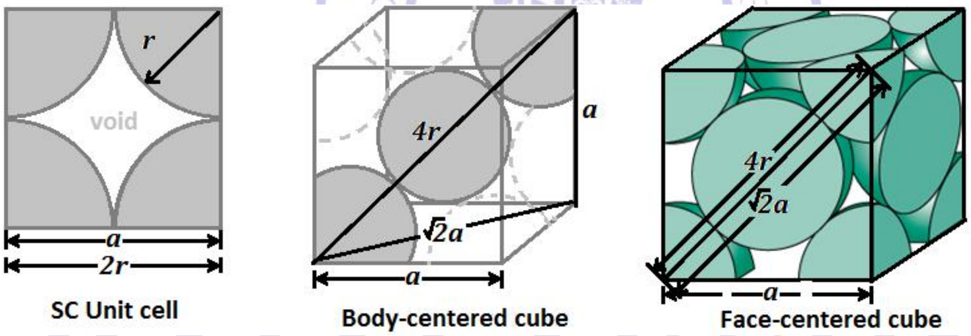


Fig. 5.9 – Cubic unit cells

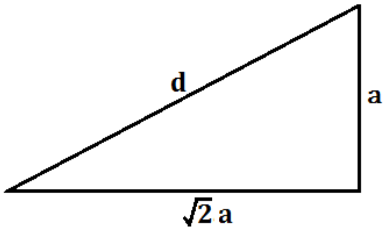
Packing Fraction of a Body-centered Cubic Unit Cell

In a body-centered lattice, adjacent atoms *touch* each other along the body diagonal of the unit cell (see figure).

If the sides of the unit cell are '*a*', then its face diagonal will be $\sqrt{2a}$ (by Pythagoras theorem) and its body diagonal will be $\sqrt{3a}$ (using Pythagoras theorem again) as shown below:

$$d^2 = a^2 + \left(\sqrt{2}a\right)^2$$

$$d^2 = 3a^2$$



Therefore,

$$d = \sqrt{3}a$$

Three atoms lie along the body diagonal with the total length being equal to *4r*. Thus we have,

$$4r = \sqrt{3}\,a$$

Or,

$$r = \frac{\sqrt{3}}{4}a$$

Hence the atomic packing fraction can be calculated as below:

$$APF = \frac{N \times V_{atom}}{V_{unit\,cell}} = \frac{2 \times \left(\frac{4}{3}\pi r^3\right)}{a^3}$$

Using the a-r relation, we get,

$$APF = \frac{2\left(\frac{4}{3}\pi\left(\frac{\sqrt{3}\,a}{4}\right)^3\right)}{a^3} = \frac{\pi\sqrt{3}}{8}$$

Or,

$$APF = \frac{\pi\sqrt{3}}{8} \cong 0.68$$

Thus the packing fraction of a body-centered cubic lattice is 0.68 or 68%. This means that only 52% of the volume is occupied by atoms and the remaining 32% is empty (void).

Packing Fraction of a Face-centered Cubic Unit Cell

In a face-centered cubic lattice, adjacent atoms 'touch' each other along the face diagonal of the cubic unit cell (see figure).

If the side length of the cube is 'a' then the length of the face diagonal will be $\sqrt{2}a$ (by Pythagoras theorem).

Therefore we have,

$$4r = \sqrt{2}a$$

Or,

$$r - \frac{a}{2\sqrt{2}}$$

Hence the atomic packing fraction can be calculated as below:

$$APF = \frac{N \times V_{atom}}{V_{unit\,cell}} = \frac{4 \times \left(\frac{4}{3}\pi r^3\right)}{a^3}$$

Using the a-r relation, we get,

$$APF = \frac{4\left(\frac{4}{3}\pi\left(\frac{a}{2\sqrt{2}}\right)^3\right)}{a^3} = \frac{\pi}{3\sqrt{2}}$$

Or,

$$APF = \frac{\pi}{3\sqrt{2}} \cong 0.74$$

Thus the packing fraction of a body-centered cubic lattice is 0.74 or 74%. This means that 74% of the volume is occupied by atoms and the remaining 26% is empty (void).

It can be noted that the FCC structure has the highest packing fraction among the cubic structures. In fact, it is also the highest APF among all the Bravais lattices along with the HCP structure which also has the same APF of 74% (as will be shown in the next section).

Packing Fraction of a Hexagonal Close Packed Unit Cell

Hexagonal close packed lattice has alternating hexagonal layers offset from each other such that any lattice point in a layer is exactly above or below the centroid of the three lattice points below or above it.

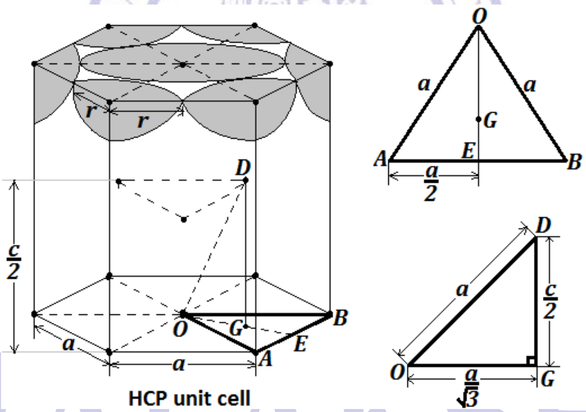


Fig. 5.10 – HCP unit cell

In an HCP unit cell we thus find three layers: hexagonal, triangular, and hexagonal. If the side length of the unit cell is *‘a’* and its height is *‘c’*, then the triangular layer will be positioned exactly at a height of c/2 from the bottom layer (as well as the top layer; see figure).

The foot of perpendicular dropped from any one of the lattice point (D) in the triangular layer will meet the bottom hexagonal layer at the centroid (G) of one of the six equilateral triangles (OAB) making it.

Adjacent atoms touch along the unit cell sides and so we have,

$$2r = a$$

Or,

$$r = \frac{a}{2}$$

Axial Ratio (c/a)

We are first interested in finding the axial ratio (the value of c/a) of the HCP unit cell, in order to calculate its packing fraction.

Let us first find the length OG.

In the equilateral triangle OAB, OG lies along the altitude OE.

Length of OE can be calculated using the Pythagoras theorem, for the right triangle OAE:

$$AE^2 + OE^2 = OA^2$$

Or,

$$OE^2 = OA^2 - AE^2 = a^2 - \left(\frac{a}{2}\right)^2 = \frac{3a^2}{4}$$

Therefore, the altitude OE is given as,

$$OE = \frac{\sqrt{3}\,a}{2}$$

Since G is the centroid of the triangle OAB,

$$OG = \frac{2}{3} OE$$

Due to the property of centroid (that a centroid cuts the median in the ration 2:1; that is OG:GE = 2:1)

Thus we have,

$$OG = \frac{2}{3} \times \frac{\sqrt{3}}{2} a = \frac{a}{\sqrt{3}}$$

Using the above value, we can calculate the axial ration (c/a) by once again applying Pythagoras theorem to the right triangle ODG:

$$OG^2 + DG^2 = OD^2$$

That is,

$$\left(\frac{a}{\sqrt{3}}\right)^2 + \left(\frac{c}{2}\right)^2 - a^2$$

(Note: OD = a, since two atoms touch along that length; since a = 2r)

Simplifying,

$$\frac{a^2}{3} + \frac{c^2}{4} = a^2$$

Or,

$$\frac{c^2}{4} = \frac{2a^2}{3}$$

And so we have,

$$\frac{c^2}{a^2} = \frac{8}{3}$$

Or,

$$\frac{c}{a} = \sqrt{\frac{8}{3}} \cong 1.63$$

Thus the axial ration (c/a) of a hexagonal close-packed lattice is $\sqrt{8/3}$ or 1.63.

Packing Fraction

We can now proceed to calculate the atomic packing fraction of the HCP unit cell.

We know that,

$$APF = \frac{N \times V_{atom}}{V_{unit\ cell}} = \frac{6 \times \left(\frac{4}{3}\pi r^3\right)}{V_{unit\ cell}}$$

The volume of the hexagonal unit cell ($V_{unit\ cell}$) can be determined as following:

$$V_{unit\ cell} = c \times \text{base area}$$

The base of the HCP unit cell is a regular hexagon of side *‘a’*, which can be considered to be made of 6 equilateral triangles of side *‘a’*, thus we have,

$$\text{base area} = 6 \times \left[\frac{1}{2} \times \text{base} \times \text{height}\right]_{\text{equilateraltriangle}}$$

$$= 6 \times \frac{1}{2} \times a \times \frac{\sqrt{3}}{2} a$$

$$= \frac{3\sqrt{3}}{2} a^2$$

Thus the volume of the unit cell is given as,

$$V_{unit\ cell} = c \times \frac{3\sqrt{3}}{2} a^2$$

Using $c/a = \sqrt{8/3}$, the above relation simplifies to,

$$V_{unit\ cell} = 3\sqrt{2} \cdot a^3$$

The atomic packing fraction, therefore, can be calculated as below,

$$APF = \frac{6 \times \left(\frac{4}{3}\pi r^3\right)}{3\sqrt{2} \cdot a^3}$$

Using r = a/2 and simplifying, we get,

$$APF = \frac{6 \times \left(\frac{4}{3}\pi \left(\frac{a}{2}\right)^3\right)}{3\sqrt{2} \cdot a^3} = \frac{\pi}{3\sqrt{2}}$$

Or,

$$APF = \frac{\pi}{3\sqrt{2}} \cong 0.74$$

Thus the packing fraction of a HCP lattice is 0.74 or 74%. This means that 74% of the volume is occupied by atoms and the remaining 26% is empty (void).

As noted before both FCC and HCP lattices have the same packing fraction of 74% which is also the highest among the Bravais lattices.Considering the fact that both these lattices also have the same coordination number (12) we realize that these two are very similar to each other.

In fact, they are both formed by stacking alternating hexagonal layers. While HCP consists of only two alternating layers (ABABAB...) the FCC lattice consists of three alternating layers (ABCABCABC...) leading to the apparent difference in unit cell shape and structure while having the same coordination number and packing fraction.

This is illustrated in the figure below:

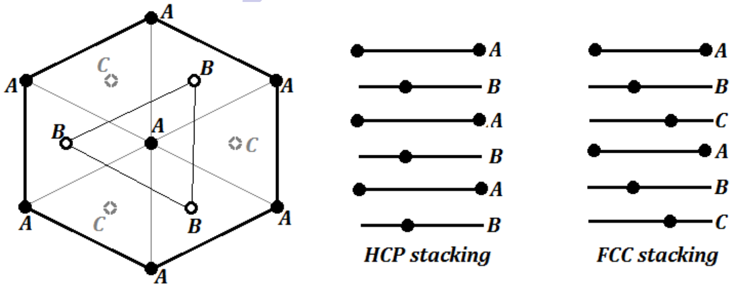


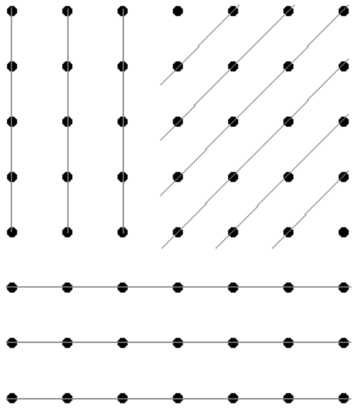
Fig. 5.11 – Stacking in HCP and FCC lattices

5.10 DIRECTIONS AND PLANES IN CRYSTALS

Since crystals have a well defined regular and periodic arrangement of atoms they are anisotropic. That is, a given physical property (conductivities, elastic modulus, refractive index, etc) of a crystal depends on the direction in which it is measured along the crystal.

Hence it becomes necessary to identify the orientation of unit cells in a macroscopic crystal specimen. We shall first develop a system of identifying and labeling the various directions inside a crystal.

Lattice points of a crystal can be considered to be lying in sets of parallel planes in various ways (infinite ways!) Any set of lattice points lying within a chosen plane, there can always be found a set of parallel planes, consisting of adjacent lattice points. This is shown below for a 2-dimensional lattice as a example.



ig. 5.12 – Lattice planes

Hence it is adequate to identify and label such sets of parallel planes to deal with the orientations of a crystal lattice - the directions inside a lattice will be identified as being normal to these parallel plane sets.

Such a labeling system is known as Miller indices.

5.11 MILLER INDICES

Miller indices are a set of three integers that uniquely identify a given set of parallel planes and the direction normal to them within a crystal lattice.

Miller indices are denoted by the notation (h k l) where ‘h’, ‘k’, and ‘l’ are integers corresponding to the axial intercepts of a given plane set. The direction normal to that set of parallel planes will be denoted by the notation [h k l]

(Note: Miller indices referring to a set of parallel planes are enclosed in parenthesis ‘(‘ & ‘)’ with only a space separating them and not commas, hyphens or dots. The direction associated with that set of planes is denoted by using the same integers enclosed in square brackets ‘[‘& ‘]’. Miller indices enclosed in ‘{‘& ‘}’ refer to a family of planes.)

Finding the Miller Indices of a Given Plane

Miller indices are basically the reciprocal of the axial intercepts of a given plane. To determine the Miller indices of a plane we have to first choose a convenient origin for the axis system of the crystal lattice.

Next, we find the axial intercepts of the given plane on all the three axes.

These will be integer multiples of the unit cell dimensions (a, b, & c) along the respective axes. We then divide the axial intercepts by these unit cell dimensions to get the axial intercepts as integers (p, q, & r).

These integers are then reciprocated $\left(\frac{1}{p},\frac{1}{q},\frac{1}{r}\right)$and brought to be another set of integers by multiplying with their LCM.

The resulting set of integers (h k l) will be the Miller indices of a given plane and the set of all planes parallel to it.

The steps to find the Miller indices are summarized below:

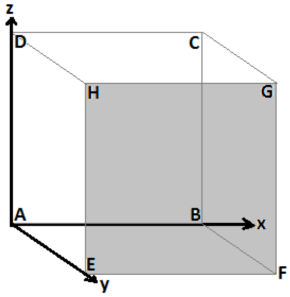
Step – 1: Find the axial intercepts ($x, y, z \rightarrow pa, qb, rc$)

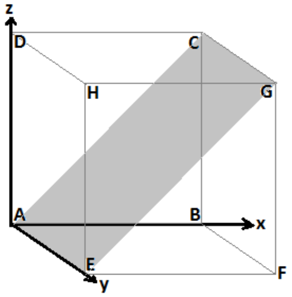
Step – 2: Divide them by unit cell dimensions $\left(\frac{pa}{a},\frac{qb}{b},\frac{rc}{c}\right)$

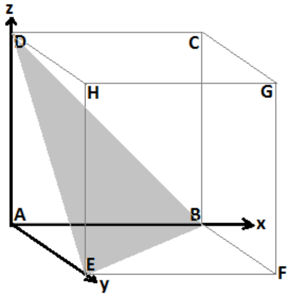
Step – 3: Find their reciprocals $\left(\frac{1}{p},\frac{1}{q},\frac{1}{r}\right)$

Step – 4: Multiply with their LCM to get (h k l)

The above process is illustrated below for some of the planes in a cubic lattice:







Plane:	**EFGH**	**ACEG**	**BDE**
Intercepts (x, y, z):	∞, a, ∞	a, ∞, a	a, a, a
Reciprocal:	$\frac{1}{\infty},\frac{1}{a},\frac{1}{\infty}$	$\frac{1}{a},\frac{1}{\infty},\frac{1}{a}$	$\frac{1}{a},\frac{1}{a},\frac{1}{a}$
Miller Indices:	(0 1 0)	(1 0 1)	(1 1 1)

Note: The Miller index corresponding to an axis which is parallel to a given plane will be zero (‘0’).

In the above illustration, we can note that the Miller indices for planes forming the **faces** of the cube will all have one ‘1’ and two ‘0’s ((100),(010),(001), etc). Without a rigid choice of axes these planes are all similar macroscopically and thus are referred to collectively as a ‘***family of planes***’, their Miller indices being denoted by {h k l} ({1 0 0} for the above mentioned family!)

To identify / sketch a lattice plane from its Miller indices we use the same process in reverse. That is, reciprocate the Miller indices, multiply with their LCM to get integers, and then finally multiply with the corresponding unit cell lengths to get the axial intercepts. Use these to sketch the plane in its proper coordinate system.

Illustration:

Forward: Finding Miller Indices

Axial intercepts : 2a, 3b, 4c
Integers : 2, 3, 4
Reciprocals : 1/2, 1/3, 1/4
Multiply with LCM : 12/2, 12/3, 12/4
Miller indices : (6 4 3)

Reverse: Finding the Plane Using Miller Indices

Miller indices : (6 4 3)
Reciprocals : 1/6, 1/4, 1/3
Multiply with LCM : 12/6, 12/4, 12/3
Integers : 2, 3, 4
Axial intercepts : 2a, 3b, 4c

Inter-Planar Spacing (d – Spacing):

Miller indices of a given set of lattice planes can be correlated to the separation between the adjacent planes of that set (interplanar spacing or d-spacing) and thus can be used to correlate the orientation of unit cell in a crystal to its macroscopic specimen (by finding the interplanar spacing in a given direction of the specimen experimentally using tools like X-ray diffraction studies!)

Let us consider a cubic lattice and two planes, nth and (n+1)th from the origin (ABC and EFG), from a set of parallel planes denoted by the Miller indices (h k l) (See figure). The planes are situated at a distance of ‘d_n’ and ‘d_{n+1}’ from the origin respectively. We shall determine these distances ‘d_n’ and ‘d_{n+1}’ first, using Miller indices, and then the separation between the planes, which will be given by,

$$d = d_{n+1} - d_n$$

Since the Miller indices of these planes are (h k l) the axial intercept on a given axis will be an integer multiple of the product of the corresponding Miller index and the unit cell parameter along that axis.

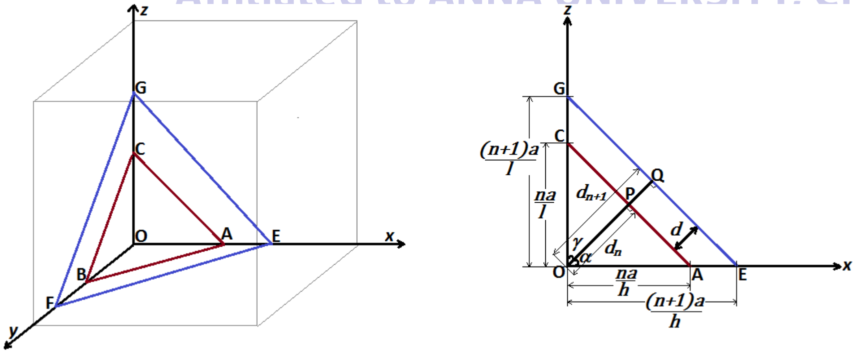


Fig. 5.13 – Identifying Miller indices

For the nth plane:

The axial intercepts for the nth plane can be written as below:

$$OA = n\frac{a}{h}, OB = n\frac{a}{k}, \quad OC = n\frac{a}{l}$$

Let $\overrightarrow{d_n}$ be the normal of this plane passing through the origin (that is, $\overrightarrow{d_n}$ is the position vector of the plane). Let *α, β,* and *γ* be the angles between the normal and the *x, y,* and *z* axes respectively (see figure).

According to the cosine law (for directional cosines), we have,

$$\cos^2\alpha + \cos^2\beta + \cos^2\gamma = 1$$

From triangle OAP,

$$\cos\alpha = \frac{d_n}{\left({}^{na}/_{h}\right)} = \frac{d_n h}{na}$$

Similarly, from triangles OBP and OCP,

$$\cos\beta = \frac{d_n k}{na}$$

And,

$$\cos\gamma = \frac{d_n l}{na}$$

Substituting these in the cosine law, we have,

$$\left(\frac{d_n h}{na}\right)^2 + \left(\frac{d_n k}{na}\right)^2 + \left(\frac{d_n l}{na}\right)^2 = 1$$

Or,

$$\frac{d_n^2}{n^2a^2}(h^2 + k^2 + l^2) = 1$$

Therefore,

$$d_n^2 = \frac{n^2a^2}{(h^2 + k^2 + l^2)}$$

Or,

$$d_n = \frac{na}{\sqrt{(h^2 + k^2 + l^2)}}$$

For the (n+1)th plane:

Proceeding as above for the next plane, we have,

The axial intercepts,

$$OE = (n+1)\frac{a}{h}, OF = (n+1)\frac{a}{k}, \quad OG = (n+1)\frac{a}{l}$$

If $\vec{d}_{n+1}$ be the normal to this plane making angles *α'*, *β'*, and *γ'* with the axes respectively, then, the cosine law can be written as,

$$\cos^2\alpha' + \cos^2\beta' + \cos^2\gamma' = 1$$

From triangles OEQ, OFQ and OGQ, we have,

$$\cos\alpha' = \frac{d_{n+1}}{\left({(n+1)a}/{h}\right)} = \frac{d_{n+1}h}{(n+1)a}$$

And,

$$\cos\beta' = \frac{d_{n+1}k}{(n+1)a}$$

$$\cos\gamma' = \frac{d_{n+1}l}{(n+1)a}$$

Hence we have, from cosine law,

$$\left(\frac{d_{n+1}h}{(n+1)a}\right)^2 + \left(\frac{d_{n+1}k}{(n+1)a}\right)^2 + \left(\frac{d_{n+1}l}{(n+1)a}\right)^2 = 1$$

Or,

$$\frac{d_{n+1}^2}{(n+1)^2a^2}(h^2+k^2+l^2) - 1$$

And so,

$$d_{n+1} = \frac{(n+1)a}{\sqrt{(h^2+k^2+l^2)}}$$

Subtracting (1) from (2), we get the distance between the two adjacent planes as,

$$d = d_{n+1} - d_n = \left(\frac{(n+1)a}{\sqrt{(h^2+k^2+l^2)}}\right) - \left(\frac{na}{\sqrt{(h^2+k^2+l^2)}}\right)$$

$$d = \frac{a}{\sqrt{(h^2+k^2+l^2)}}$$

The above is the required expression for the inter-planar spacing of a set of lattice planes denoted by the Miller indices (h k l), with unit cell dimension *'a'*.

Note: This relation applies only for the cubic lattices. For non-cubic lattices, we have to use a, b, and c in writing equation () instead of all 'a'. Such relations do not simplify to a compact form as above but are nevertheless necessary to deal with those lattices.

5.12 DIFFRACTION BY CRYSTALS

X-rays are electromagnetic radiation with wavelengths between about 0.02 Å and 100 Å (1 Å = 10^{-10} meters). The wavelength of X-rays is on an atomic level and is much smaller than that of visible light (3000 to 8000 Å). Since X-rays have a smaller wavelength than visible light, they have higher energy and are more penetrative. Its ability to penetrate matter, however, is dependent on density of the matter. Therefore, X-rays are useful in exploring structures of atoms.

One of the best methods of determining a crystal's structure is by X-ray diffraction. In macromolecular x-ray diffraction experiments, an intense beam of X-ray strikes the crystal of study. In general, crystal diffracts the X-ray beam differently, depending on its structure and orientation. The diffracted X-ray is collected by an area detector. The diffraction pattern consists of reflections of different intensity which can be used to determine the structure of the crystal. However, many different orientations of the crystal need to be collected before the true structure of the crystal can be determined.

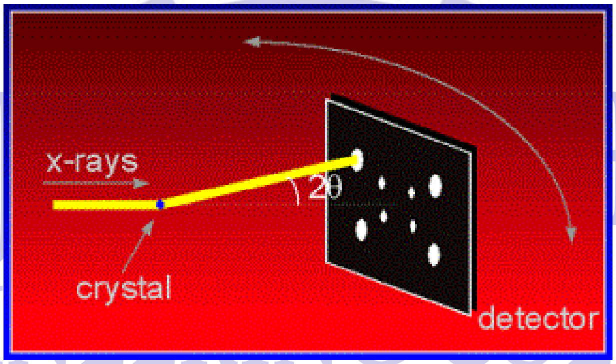


Figure 5.14 Diffraction of X-rays by crystal

The resolution of an X-ray diffraction detector is determined by the Bragg equation:

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

The setup of an X-ray detector is shown in the following:

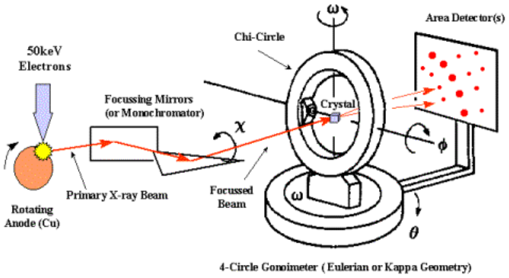


Figure 5.15 Sketch of X-ray detector

The atoms in crystals interact with X-ray waves in such a way as to produce interference. Because crystal structures contain planes of atoms, each plane will reflect incident X-rays differently. For example, let two monochromatic X-ray beams (of a specific wavelength) strike a crystal structure at an incoming angle of *theta*. Ray 1 will reflect off of the top atomic plane while Ray 2 will reflect from the second atomic plane. However, because Ray 2 has to cross deeper into the atomic plane, it travels a distance 2a farther than Ray 1. If the distance 2a is equal to the integral number (n**lambda*) of wavelength of two waves, then Ray 1 and 2 will be in phase, thus constructively interfere, when they both exit the crystal.

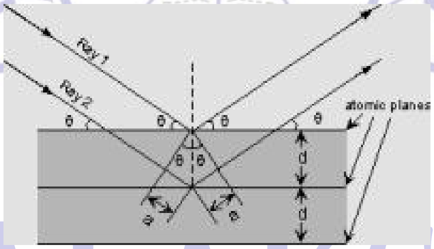


Figure 5.16 Braggs' Law

From Bragg's law, we know that n**lambda* = 2*d* sin theta, therefore if we know the wavelength *lambda* of the X-rays going in to the crystal, and we can measure the angle *theta* of the diffracted X-rays coming out of the crystal, then we can determine the spacing between the atomic planes. This spacing is the called the d-spacing. If we now reorient the crystal to a different atomic plane, we can measure the d-spacing in other planes. By doing multiple x-ray diffractions at different crystal orientations, we can determined crystal structure and the size of the unit cell of the crystal.

The Powder Method

Practically speaking, reorienting the crystal to every plane and measuring the diffraction angle *theta* to determine the d-spacing of each plane is very time consuming. Thus, the powder method is often used to speak up the process. In this method, the crystal of study is ground into fine powder. The find powder contains small granules of crystals with random orientations. If we have enough powder randomly oriented on the surface, we expect some of the different atomic planes to lie parallel to the surface. Therefore, if we scatter an incident X-ray beam from 0 to 90 degrees, we should find all the angles where diffraction occurred.

Each of these angles will correspond to a different atomic spacing. The instrument used to make these measurements is the X-ray powder diffractometer. To rotate both the X-ray tube and the detector through the 90 degrees angle, a goniometer is used.

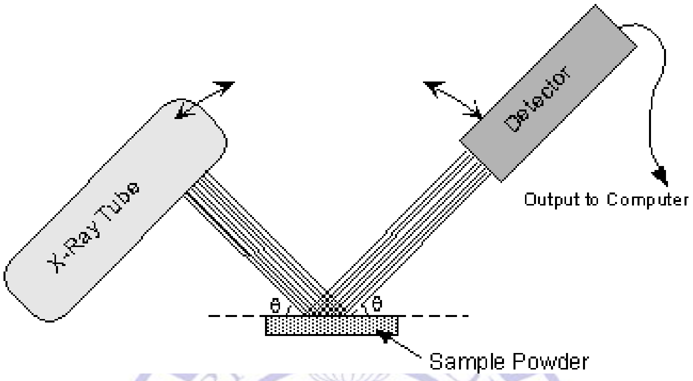


Figure 5.17 Schematic sketch of powder X-ray setup

The data recorded in the detector is the X-ray intensity in counts/second. By plotting the intensity against the angle of the incident X-ray, we can produce a series of peaks. These diffraction peaks correspond to d-spacing and can be converted using the Bragg equation.

Interpretation of diffraction peaks

The powder x-ray diffraction pattern for a given material can be used to determine unit cell dimensions and that can be correlated to inter-atomic distances. Any changes in inter-atomic distances arising as a result of temperature, doping and stress will be reflected by a change in peak positions.

To calculate unit cell dimensions from diffraction peak positions, follow the below steps:

1. Convert the peak positions, 2 theta into d_{hkl} values using Bragg's law:
$$d_{hkl} = \lambda / 2 \sin\theta$$

2. Determine the Miller indices (hkl) of the diffraction peaks from the published reference pattern – If you do not have access to a reference pattern that identifies (hkl) then you will need to index the pattern to determine the (hkl) using available software.

3. Use the d^{*2} equation to calculate the lattice parameters – Most analysis programs contain an unit cell refinement algorithm for numerically solving the lattice parameters – These programs can also calculate and correct for peak position error due to specimen displacement.

$$d^{*2}_{hkl} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^* + 2hla^*c^*\cos\beta^* + 2klb^*c^*\cos\alpha^*$$

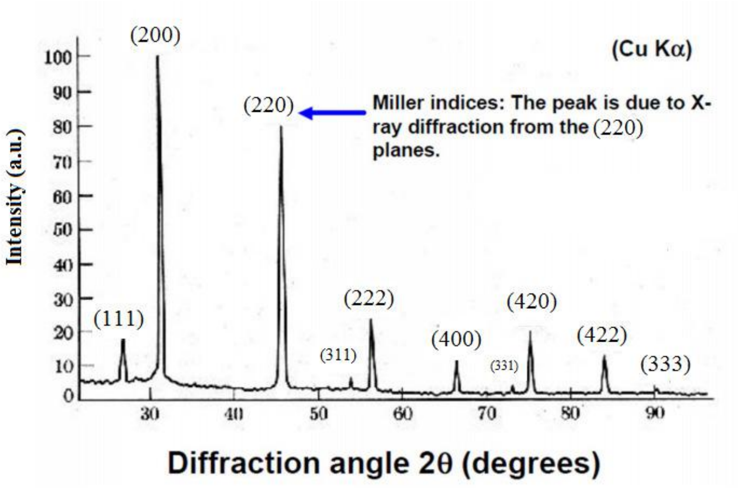


Figure 5.18 Powder X-ray diffractogram of NaCl crystalline sample

5.13 RECIPROCAL LATTICE

Crystal structures are analysed by diffraction studies. Diffraction is usually performed using X-rays, electron, or neutron beams. Such diffraction is governed by the Bragg's law:

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

Where *'d'* in the interplanar spacing. It is the shortest distance between any two planes in a set of parallel planes, referred to by the Miller indices (h k l), and hence 'd' can be denoted as d_{hkl} as well.

Through any given point in a crystal lattice many set of parallel planes can be considered. The incident beam may be diffracted by all such planes and hence the situation becomes complex to deal with in the direct lattice space.

However, we can represent a set of parallel planes by their normal (notice that there is only one normal to all the planes in a set of parallel planes!) and so reduce the complexity of visualizing the diffraction. Since the diffraction peak depends on the interplanar spacing (d_{hkl}) we can set the length of the normal of the planes (h k l) to be the reciprocal of d_{hkl}.

Thus we construct a dual lattice with points representing set of planes in the direct lattice known as the reciprocal lattice (since distances in this lattice has the dimensions of inverse length [L^{-1}]).

The reciprocal lattice is constructed in the following way:

1. Choose a convenient origin in the direct lattice (this can be any valid lattice point)
2. Identify the planes (h k l) passing through this origin and draw normals to all the planes.
3. Set the length of the normals to be 1/ d_{hkl}
4. Points at the end of all these normals corresponds to the reciprocal space.

Notice that each point in the reciprocal space corresponds to a set of parallel planes in the direct lattice.

Alternatively, we can use vector notation to construct the reciprocal lattice space.

If **a**, **b**, and **c** are the primitive vectors of a direct lattice (that is, the position of any lattice point in that lattice, from a suitable origin, can be written as $\mathbf{R} = p\mathbf{a} + q\mathbf{b} + r\mathbf{c}$, where p, q and r are integers), the primitive vectors of the corresponding reciprocal lattice is written as:

$$\mathbf{a}^* = (2\pi/V)\, \mathbf{b} \times \mathbf{c}$$

$$\mathbf{b}^* = (2\pi/V)\, \mathbf{c} \times \mathbf{a} \text{ and}$$

$$\mathbf{c}^* = (2\pi/V)\, \mathbf{a} \times \mathbf{b}$$

Where $V = \mathbf{a} \cdot (\mathbf{b} \times \mathbf{c})$ is the volume of the unit cell.

The factor '2π' is used by Physicists. Crystallographers usually omit it.

We have this factor since the reciprocal lattice can also be written as the Fourier transform of the direct lattice.

In a lattice with periodicity 'a' (along one dimension, say 'x') any physical quantity, such as electron density, will also have the same periodicity 'a', that is:

$$n(x) = n(x+a)$$

We can write this periodic function as a Fourier series,

$$n(x) = n_0 + \sum_{p>0} \left[C_p \cos\left(\frac{2\pi p x}{a}\right) + S_p \sin\left(\frac{2\pi p x}{a}\right) \right]$$

where '*p*' are positive integers and C_p and S_p are real constants, known as the Fourier coefficients.

The factor 2π/a ensures that n(x) has the period a.

We can say that 2πp/a is a point in the reciprocal lattice or Fourier space of the crystal.

Reciprocal Lattice of a Simple Cubic Lattice:

The primitive vectors of a simple cubic lattice can be written as follows:

$$\boldsymbol{a} = a\hat{x}$$

$$\boldsymbol{b} = a\hat{y}$$

$$\boldsymbol{c} = a\hat{z}$$

And so, the reciprocal lattice vectors will be,

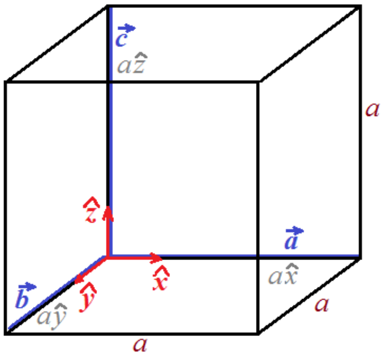


Fig: Primitive vectors of a SC lattice

$$a^* = \left(\frac{2\pi}{a^3}\right) b \times c = \left(\frac{2\pi}{a^3}\right) (a\hat{y} \times a\hat{z})$$

$$a^* = \left(\frac{2\pi}{a^3}\right) a^2 (\hat{x})$$

$$a^* = \frac{2\pi}{a}\hat{x}$$

Similarly,

$$b^* = \frac{2\pi}{a}\hat{y}$$

$$c^* - \frac{2\pi}{a}\hat{z}$$

Thus the reciprocal lattice of a simple cubic lattice is another simple cubic lattice with lattice constant (2π/a).

Reciprocal Lattice of a Body Centred Cubic Lattice:

The primitive vectors of a body centred cubic lattice can be written as below:

$$a = \frac{a}{2}(-\hat{x} + \hat{y} + \hat{z})$$

$$b = \frac{a}{2}(\hat{x} - \hat{y} + \hat{z})$$

$$c = \frac{a}{2}(\hat{x} + \hat{y} - \hat{z})$$

And so, the reciprocal lattice vectors will be,

$$a^* = \left(\frac{2\pi}{a^3/2}\right) b \times c$$

Where the volume of the primitive cell is $a^2/2$ (Remember, V = **a**.(**b** x **c**))

And so,

$$a^* = \left(\frac{2\pi}{a^3/2}\right)\left[\frac{a^2}{4}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{vmatrix}\right]$$

Therefore,

$$a^* = \left(\frac{2\pi}{a}\right)(\hat{y} + \hat{z})$$

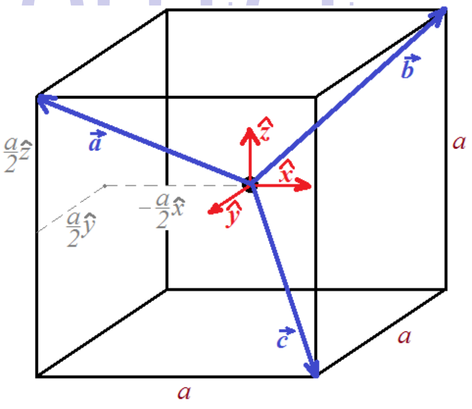


Fig: Primitive vectors of a BCC lattice

Similarly,

$$b^* = \left(\frac{2\pi}{a}\right)(\hat{z} + \hat{x})$$

$$c^* = \left(\frac{2\pi}{a}\right)(\hat{x} + \hat{y})$$

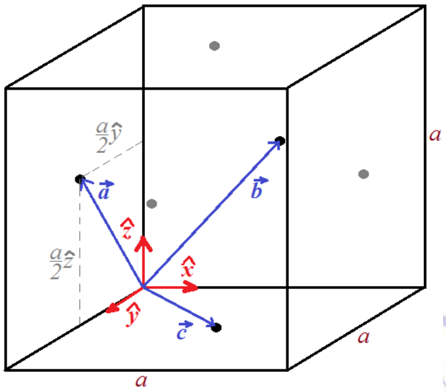


Fig: Primitive vectors of a FCC lattice

Which are the primitive vectors of a Face Centred Cubic (FCC) lattice.

Thus the reciprocal lattice of a BCC lattice is an FCC lattice with lattice constant (2π/a).

Similarly, it can be shown that the reciprocal lattice of an FCC lattice is a BCC lattice.

It should be noted that the diffraction pattern of a crystal will be a map of the reciprocal lattice of a crystal. However, the relative intensity of the diffracted spots will be given by a function known as the form factor.

5.14 CRYSTAL GROWTH

Crystallisation is the natural or artificial process in which solid crystals are formed by the precipitation from a solution or more rarely deposited directly from a gas.
It is also a chemical solid-liquid seperation technique,in which transformation of asolute from the liquid solution to a pure solid crystalline phase takes place.
Solidification, is a phase transition in which a liquid turns in to a solid when its temperature is lowered below its freezing point.
Thermodynamically,both liquid and solid have equal energy at melting point and therfore both are equally stable at melting point.During freezing the liquid changes in to solid by releasing heat.The energy released upon freezing is a latent heatand is the entropy part.
Solidification occurs by two process:nucleation and growth.
The figure shown below explains the cooling curve of the material under solidification process.

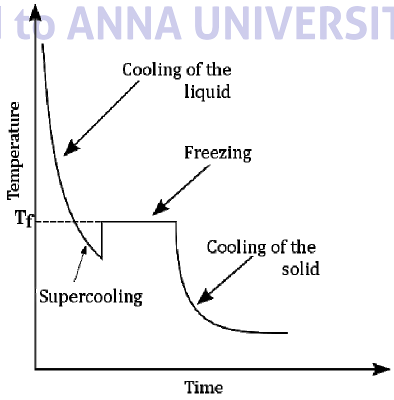


Fig. 5.19 – Cooling curve

TYPES OF CRYSTAL GROWTH

The crystal growth technique is classified in to six categories namely,

- Melt growth
- Low temperature solution growth
- High temperature solution growth
- Hydrothermal growth
- Gel growth
- Epitaxial growth

MELT GROWTH TECHNIQUES

Melt growth is the process of crystallization by fusion and resolidification process.

The main techniques are:

- Czochralski technique
- Bridgman technique

CZOCHRALSKI TECHNIQUE

This method was developed in 1916, and widely adopted to grow III-IV compound semiconductors.

In this method, the material to be grown is taken in a non-reacting container called crucible and heated under a controlled atmosphere above the melting point. A rod with chuck can de pulled contains a seed crystal at the lower end is kept above the crucible. The seed is dipped into the melt and the temperature is adjusted until a meniscus can be supported by the crystal. Then the rod is rotated and lifted slowly.

Crystal of desired diameter is grown by adjusting the power supplied to the melt. The crystal can be visually observed by placing the whole setup in an envelope with ambient gas atmosphere.

The crystal shape is free from defects because of the shape of the crucible. The rate of pulling depends on latent heat of fusion of charge, thermal conductivity, and rate of cooling of pulling rod. By adjusting the pull and rotation rate a good and uniform crystal can be obtained.

LEC is an abbreviation of liquid encapsulated czochralski technique by which a single crystal of components that produce high vapour pressure at the melting point can be grown.

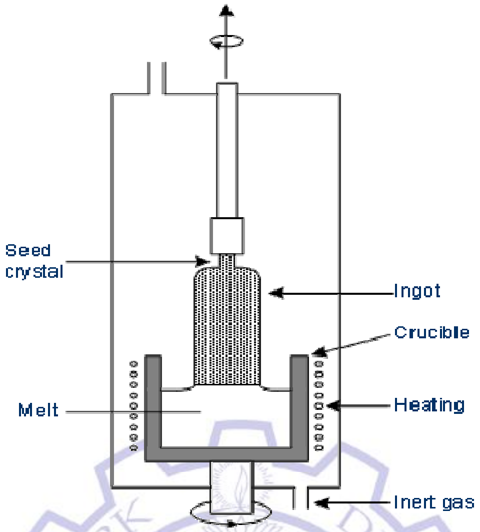


Fig. 5.20 – Melt pulling

Advantages:

The crystal without any stress can be obtained by this method since there is no direct contact between the crucible walls and crystal.

At any stage of growth crystal can be extracted from the melt and investigation on the study of growing condition can be done.

Disadvantages:

It is difficult to maintain thermodynamic equilibrium between the vapour and the melt.

Engineering problems like rotating and pulling the crystal also to be considered.

BRIDGMAN METHOD

In Bridgman technique, the crucible is a vertical cylindrical container, tapered conically with a point bottom, in which a material to be melted is taken. The material in the crucible is heated in a furnace above its melting point. The melt can be progressively frozen by moving the crucible down a temperature gradient or moving the furnace over the crucible. The movement rate range from 1-30mm/hr for such process.

At the tip the crystallization begins and continues its growth from the first formed nucleus. The latent heat of solidification is removed by conduction through the crystal and the crucible.

A wide range of substance like metallic, organic and a number of dielectric single crystals such as oxides, flurides, sulphides and halides can be grown by this technique. Sapphire is a single crystal can be grown.

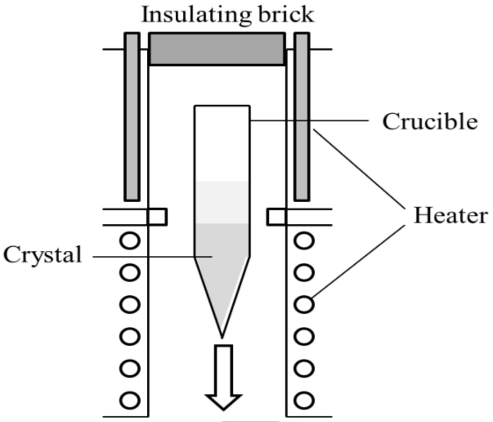


Fig. 5-21 – Bridgman technique

ADVANTAGES:

The crystal diameter can be reassigned by selecting the appropriate container.

This is a technically simple method.

5.15 CRYSTAL DEFECTS

INTRODUCTION

Crystal is never perfect. In a real crystal the lattice is not perfect, but contains imperfection or defects which explain that the perfect periodicity is disrupted in some manner. These imperfections results from deformation of the solid, rapid cooling from high temperature, or high-energy radiation (X-rays or neutrons) striking the solid. These defects may be located at single points, along lines, or on whole surfaces in the solid, influence its mechanical, electrical, and optical behavior.

The importance of defects depends upon the material, type of defect, and properties which can be considered. Certain properties like density and elastic constants are proportional to the concentration of defects, and so a small defect concentration will have a very small effect on these. Other properties, e.g. the color of an insulating crystal or the conductivity of a semiconductor crystal may be much more affected to the presence of small number of defects.

There are some properties of materials such as stiffness, density and electrical conductivity which are termed structure-insensitive, are not affected by the presence of defects in crystals while there are many properties of greatest technical importance such as mechanical strength, ductility, crystal growth, magnetic hysteresis, dielectric strength, condition in semiconductors, which are termed structure sensitive are greatly affected by the relatively minor changes in crystal structure caused by defects or imperfections.

TYPES OF IMPERFECTIONS

The various types of imperfection are defects in crystal are classified as

1. Lattice vibrations
2. Point defects
    - (a) Vacancies
    - (b) Scotty defect
    - (c) Frenkel defect
    - (d) Interstitial defects
    - (e) Substitutional Defect
3. Line defects
    - (a) Edge dislocation
    - (b) Dislocation climb
    - (c) Screw dislocation
    - (d) Dislocation slip
4. Surface defects
    - (a) Grain boundaries
    - (b) Twin boundaries
    - (c) Stacking faults
5. Volume defects

LATTICE VIBRATIONS

A type of imperfection which will be common in all crystals is atomic vibration. In perfect single crystal atoms are present at particular sites, and also assumed that the atoms separated from each other by a constant distance. The atoms in crystal have a certain thermal energy, which is a function of temperature causes the atoms to vibrate in a random manner about an equilibrium lattice point, which fluctuate the distance between the atoms and slightly disrupted the perfect geometric arrangement of atoms. This type of imperfection is called Lattice vibrations.

POINT DEFECTS

The point imperfections, which are lattice errors at isolated lattice points, take place due to imperfect packing of atoms during crystallization.

Point defects are always present in crystals and their present results in a decrease in the free energy.

(a) VACANCIES

The simplest point defect is a vacancy. This refers to an unoccupied site of a crystal lattice as shown in the figure 5.22,such defects may arise either from imperfect packing during original crystallization or from thermal vibrations of the atoms at higher temperatures.

Increase in thermal energy due to vibration will increase the probability of jumping of individual atoms out of their positions of lower energy, thereby creating a vacancy.

Vacancy may be single or divacancies or trivacancies and so on.

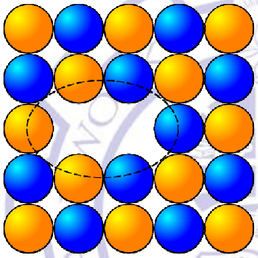


Fig. 5.22 – Vacancy

(b) SCHOTTKY DEFECTS

These imperfections are similar to vacancies. This defect is caused, whenever a pair of positive and negative ions is missing from a crystal as in the figure 5.23. This type of imperfection maintains charge neutrality.

Schottky defects are observed most frequently when there is a small difference in size between cations and anions. This defect can be created in a perfect crystal by transferring an atom from lattice site in the interior to a lattice site on the surface of the crystal. Whenever the temperature is raised above 0K the lattice suffers thermal expansion and vibration which results in the incorporation of the pair of vacancies in the crystals.

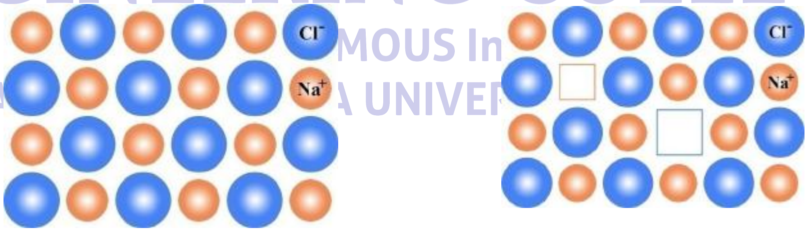


Fig. 5.23 – Defect free lattice and Schottky defect – NaCl crystal

(C) FRENKEL DEFECTS

Whenever a missing atom, which is responsible for vacancy, occupies an interstitial site as shown in figure 5.24, the defect caused is known as Frenkel defect. Frenkel defect is a combination of vacancy and interstitial defects. These defects are less in number because energy is required to force an ion into new position. This type of imperfection is more common in ionic crystals, because the positive ions, being smaller in size, get lodged easily in the interstitial positions.

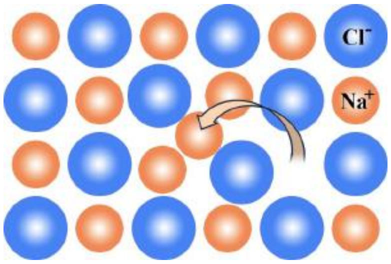


Fig. 5.24 - The Frenkel defects with in the NaCl crystal

(d) INTERSTITIAL DEFECT

In a closed packed structure of atoms in a crystal if the atomic packing factor is low, an extra atom may be blocked within the crystal structure. This is known as interstitial position, i.e. voids. An extra atom can enter the interstitial space or void between the regularly positioned atoms only when it is substantially smaller than the parent atoms as in the Figure 5.25, otherwise it will produce atomic distortion. The defect caused is known as interstitial defect. Interstitials may also be single interstitial, di-interstitials, and tri-interstitials.

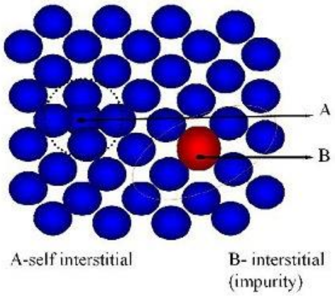


Fig. 5.25 – Interstitial defect

(e) SUBSTITUTIONAL DEFECTS

Whenever a foreign atom replaces the parent atom of the lattice and thus occupies the position of parent atom as in the Figure 5.26 the defect caused is called substitutional defect. In this type of defect, the atom which replaces the parent atom may be of same size or slightly smaller or greater than that of parent atom.

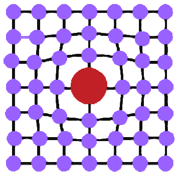


Fig. 5.26 – Substitutional defect

LINE DEFECTS

A line defect occurs when an entire row of atoms is missing from its normal lattice site. A line dislocation disrupts both the normal geometric periodicity of the lattice and the ideal atomic bonds in the crystals.

(a)EDGE DISLOCATION

An edge dislocation is the simplest one and a cross-sectional view of the atomic arrangement of atoms in it and the distortion of the crystal structure.

The Figure 5.27 shows a simple cubic crystal in which slip of one atom distance has occurred over the left half of the slip plane but over the right half.

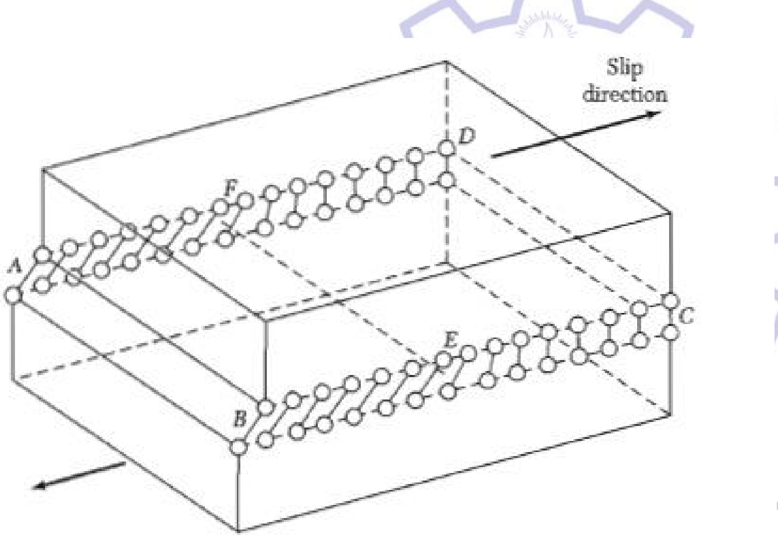


Fig. 5.27 - Dislocation

The boundary between the slipped and unslipped regions is called the dislocation. Its position is marked by the termination of an extra vertical half plane of atoms crowded in to the upper half of the crystal as in the Figure 5.28. Near the dislocation the crystal is highly strained. The simple edge dislocation extends indefinitely in the slip plane in a direction normal to the slip direction.

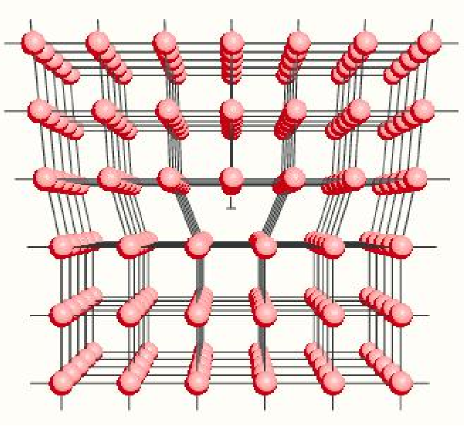
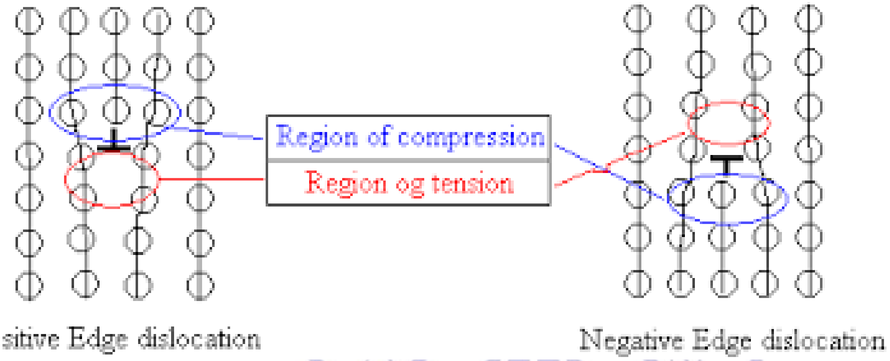


Fig. 5.28 – Edge dislocation

Edge dislocation is considered positive when compressive stresses W above the dislocation line, and is represented by ⊥. If the stress state is opposite i.e. compressive stresses exist below the dislocation line, it is considered as negative edge dislocation, and represented by ⊤.



Positive Edge dislocation

Negative Edge dislocation

(b)SCREW DISLOCATION

A screw dislocation is like a spiral ramp with an imperfection line down its axis. Screw dislocations result when displacing planes relative to each other through shear. Shear stresses are associated with the atoms adjacent to the screw dislocation; therefore extra energy is involved as it is in the case of edge dislocations. Screw dislocation is considered positive if Burger's vector and *t*-vector or parallel, and vice versa. (***t***-vector – an unit vector representing the direction of the dislocation line). A positive screw dislocation is represented by "'↻' a dot surrounded by circular direction in clock-wise direction", whereas the negative screw dislocation is represented by "'↺' a dot surrounded by a circular direction in anti-clock-wise direction" as in the Figure 5.29.

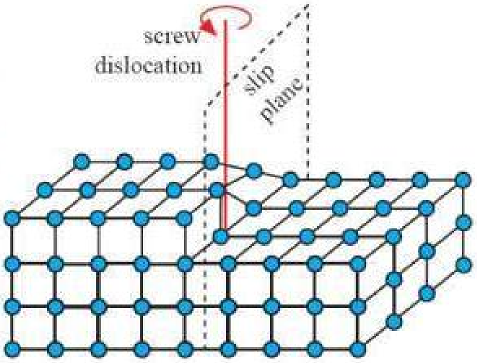


Fig. 5.29 – Screw dislocation

DIFFERENCE BETWEEN EDGE DISLOCATION AND SCREW DISLOCATION:

EDGE DISLOCATION	***SCREW DISLOCATION***
This type of dislocation arises due to the introduction or elimination of an extra row of atoms.	Additional atoms and unit cells can be added to step of the screw. So it provides for easy crystal growth.
Tensile, compressive and shear stress fields can be present.	Only the shear stress field exists.
The region of lattice disturbance extends along a dislocation line.	The region of lattice disturbance extends in two separate planes at right angles to each other.
Burger's vector is perpendicular to the dislocation line.	Burger's vector is parallel to the dislocation line.

BURGER'S VECTORS

The magnitude and the direction of the displacement are defined by a vector, called the Burgers Vector.

In figure 5.30 (a), starting from the point P, we go up by 6 steps, then move towards right by 5 steps, move down by 6 steps and finally move towards left by 5 steps to reach the starting point P. Now the Burgers circuit gets closed.

When the same operation is performed on the defect crystal (figure 5.30 (b)) we end up at Q instead of the starting point.

So, we have to move an extra step to return to P, in order to close the Burgers circuit.

The magnitude and the direction of the step define the Burgers Vector (BV).

BV = b

The Burgers Vector is perpendicular to the edge dislocation line.

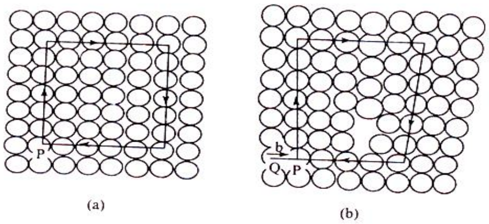


Fig. 5.30 – Burger vectors

SURFACE DEFECTS

This kind of defects can be defined as boundaries that have two dimensional imperfections in crystalline solids. These imperfections are meta-stable imperfections and they are not thermodynamically stable. It arises from the clustering of line defects in to a plane.

(a)GRAIN BOUNDARIES:

Crystalline solids which are made up of number of grains seperated by a wall or boundaries are called grain boundaries.These boundaries are several atoms distances wide and there will be a mismatch of orientation of grains on either side of the boundary as in the Figure 5.31. If the orientaion of the misalignment is slight,on the order of few degrees(<10^6) it is called low angle grain boundary.

If the low grain boundary is formed by edge dislocation then ,it is called tilt boundary.If it is formed because of screw dislocation ,then it is called twist boundary.

If the degree of disorientation is of large range(>15®) then they corresponds to ,high angle grain boundaries.

Because of grain boundary energy , grain boundaries are chemically more reactive.Polycrystalline solids are more strong bcause of cohesive force present within and across the boundary.

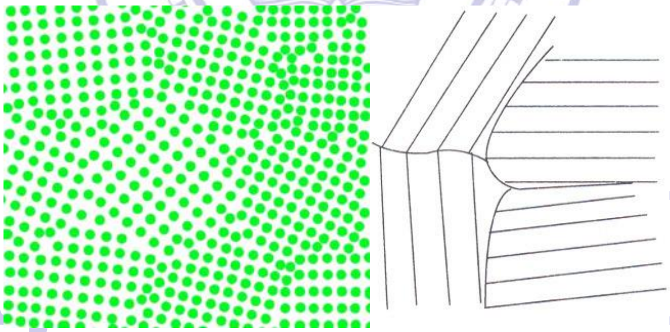


Fig. 5.31 - Schematic representation of grain boundaries.

(b) TILT BOUNDARIES

This is called low-angle boundary as the orientation difference between two neighbouring crystals is less than 10°.

The disruption in the boundary is not so high as in the high-angle boundary. In general low-angle boundaries can be described by suitable arrays of dislocation.

Actually a low-angle tilt boundary is composed of edge dislocation lying one above the other.

The angle or tilt will be

$$\theta = \frac{b}{D}$$

where b = Burgers vector and

D = the average vertical distance between dislocations.

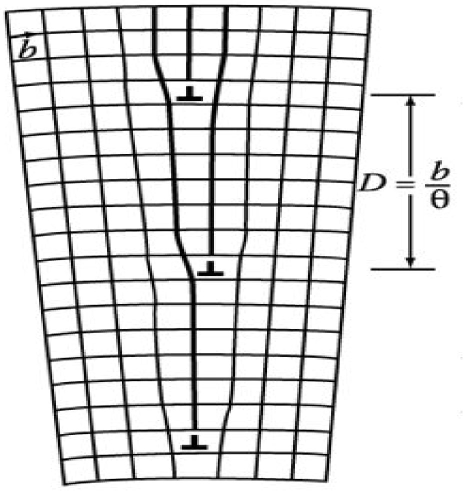


Fig. 5.32 – Tilts

(c) TWIN BOUNDARIES

In this type across the grain boundary there is specific mirror lattice symmetry.Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restore by the other as in the figure.The region between the pair of boundaries ,called as twinned region.

Annealing twins are formed during the process of recrystallisation and deformation twins forms during plastic deformation.

Annealing twins are formed in metals have FCC structure,but deformation twins formed in BCC and HC
P metals.

Annealing twins are usually broader and with straighter sides than deformation twins.These twins do not extend beyond a grain boundary.

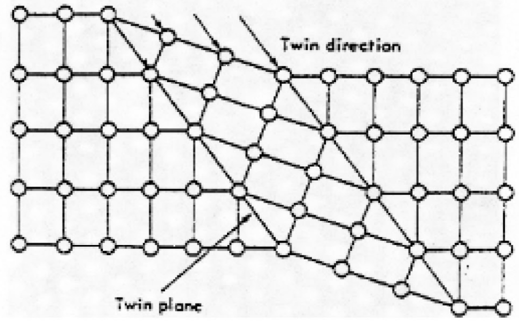


Fig. 5.33 – Twin boundaries

(d)STACKING FAULTS

Stacking faults are faults in stacking sequence of atom planes. Normal stacking sequence in an FCC crystal is ABC ABC ABC……and the sequence for HCP crystal is AB AB AB……If there is any disturbance in the stacking sequence, formation of stacking faults takes place. In FCC crystal, the two kinds of stacking faults are (a) ABC AC ABC….where CA CA represent thin HCP region which is nothing but stacking fault .(b) ABC ACB CABC is called extrinsic or twin stacking fault. The stacking faults in FCC crystal are submicroscopic twins. The range of stacking faults varies by 0.01-0.1 J/m^2.The stacking fault will be wider for lower stacking fault energy, and narrow for higher stacking energy.

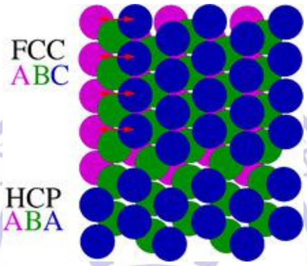


Fig. 5.34 – Stacking fault

VOLUME DEFECTS

Defects in three dimensions are called volume defects. It includes pores, cracks, foreign inclusions and other phases. Normally these defects are introduced during processing and fabrication .These defects act as a stress raisers in the material. Sometimes foreign particles are added to increase the strength of the material. Dispersion hardening, foreign particles act as obstacles to movement of dislocation, which facilitates plastic deformation.

The pores are harmful because they act as stress concentration sites which reduce effective load bearing area.

SOLVED PROBLEMS

1. Calculate the spacing between the planes (101) of a cubic crystal of side 4 Å

Solution:

Given: (h k l) = (1 0 1)

$a = 4\ \text{Å} = 4 \times 10^{-10}$ m

We know that, the interplanar spacing,

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

Therefore,

$$d_{101} = \frac{(4 \times 10^{-10})}{\sqrt{1^2 + 0^2 + 1^2}}$$

$$d_{101} = \frac{(4 \times 10^{-10})}{\sqrt{2}}$$

Thus,

$$d_{101} = 2.828 \times 10^{-10} m$$

Or,

$d_{101} = 2.828$ Å

2. Identify the crystal system that has the following unit cell parameters.

a = 4.175 Å, b = 4.175 Å, c = 4.175 Å and $\alpha = 100^0$, $\beta = 100^0$, $\gamma = 100^0$.

Solution:

The given parameters match with the parameters of the rhombohedral / trigonal crystal system for which

$a = b = c$ and $\alpha = \beta = \gamma \neq 90^0$.

Thus the crystal system is rhombohedral / trigonal.

3. Sketch the plane corresponding to the Miller indices (1 1 0) of a cubic lattice.

Solution:

Given: Miller indices (h k l) = (1 1 0)

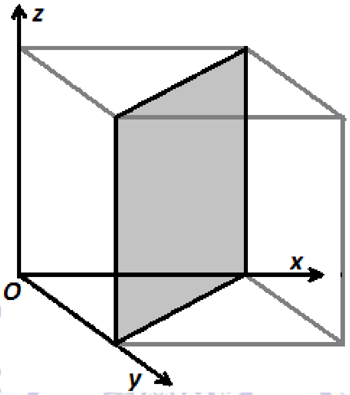
The corresponding axial intercepts can be found by reciprocating the Miller indices:

(p, q, r) = (1/h, 1/k, 1/l)

$= (1/1, 1/1, 1/0)$

$= (1, 1, \infty)$

Thus the plane with the Miller indices (110) cuts the x and y axes at unit interval and is parallel to the z axis. The plane is shown in the figure below:



Unit – III - Physics of Materials

Introduction

Materials are probably more deep-seated in our culture than most of us realize.Transportation, housing, clothing, communication, recreation, and food productionvirtually every segment of our everyday lives is influenced to one degree or anotherby materials. Historically, the development and advancement of societies have beenintimately tied to the members' ability to produce and manipulate materials to filltheir needs. In fact, early civilizations have been designated by the level of theirmaterials development (Stone Age, Bronze Age, Iron Age)

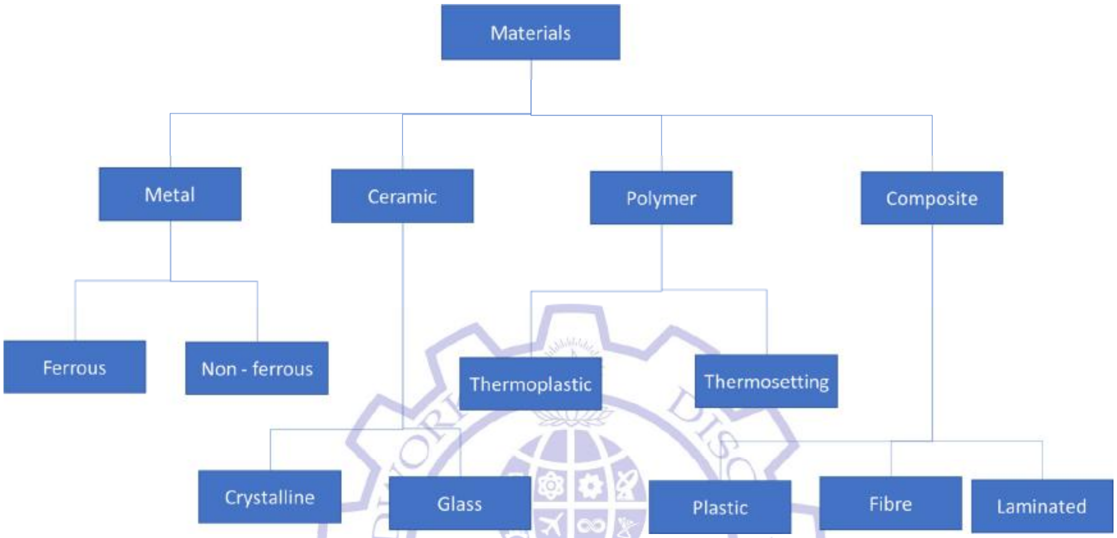
The development of many technologies that make our existence so comfort-able has been intimately associated with the accessibility of suitable materials.An advancement in the understanding of a material type is often the forerunner to the stepwise progression of a technology. For example, automobileswould not have been possible without the availability of inexpensive steel orsome other comparable substitute. In our contemporary era, sophisticated electronic devices rely on components that are made from what are called semiconducting materials.

Sometimes it is useful to subdivide the discipline of materials science and engineering into materials science and materials engineering subdisciplines. Strictlyspeaking, "materials science" involves investigating the relationships that existbetween the structures and properties of materials.

"Structure" is at this point a nebulous term that deserves some explanation. Inbrief, the structure of a material usually relates to the arrangement of its internalcomponents. Subatomic structure involves electrons within the individual atoms andinteractions with their nuclei. On an atomic level, structure encompasses the orgeneration of atoms or molecules relative to one another. The next larger structuralrealm, which contains large groups of atoms that are normally agglomerated together, is termed "microscopic," meaning that which is subject to direct observationusing some type of microscope. Finally, structural elements that may be viewed withthe naked eye are termed "macroscopic."

The four components of physics of materials and engineering

Solid materials have been conveniently grouped into three basic classifications: metals, ceramics, and polymers. This scheme is based primarily on chemical makeup andatomic structure, and most materials fall into one distinct grouping or another, although there are some intermediates. In addition, there are the composites, combinations of two or more of the above three basic materialclasses.



Classification of materials into four groups

Metals

Materials in this group are composed of one or more metallic elements (such as iron,aluminum, copper, titanium, gold, and nickel), and often also nonmetallic elements (forexample, carbon, nitrogen, and oxygen) in relatively small amounts. Atoms in metalsand their alloys are arranged in a very orderly manner

Metallic materials have large numbers ofnonlocalized electrons; that is, these electrons are not bound to particular atoms. Manyproperties of metals are directly attributable to these electrons. For example, metalsare extremely good conductors of electricity (Figure 1.7) and heat, and are not transparent to visible light; a polished metal surface has a lustrous appearance. In addition, some of the metals (viz., Fe, Co, and Ni) have desirable magnetic properties.

Ceramics

Ceramics are compounds between metallic and nonmetallic elements; they are mostfrequently oxides, nitrides, and carbides. For example, some of the common ceramic materials include aluminum oxide (or alumina,Al_2O_3), silicon dioxide (or silica, SiO_2),silicon carbide (SiC), silicon nitride (Si_3N_4), and, in addition, what some refer to asthe traditional ceramics—those composed of clay minerals (i.e., porcelain), as well ascement, and glass.

Polymers

Polymers include the familiar plastic and rubber materials. Many of them are organiccompounds that are chemically based on carbon, hydrogen, and other nonmetallicelements (viz. O, N, and Si). Furthermore, they have very large molecular structures,often chain-like in nature that have a backbone of carbon atoms. Some of the common and familiar polymers are polyethylene (PE), nylon, poly (vinyl chloride)(PVC), polycarbonate (PC), polystyrene (PS), and silicone rubber.

ADVANCED MATERIALS

Materials that are utilized in high-technology (or high-tech) applications are sometimes termed advanced materials. By high technology we mean a device or productthat operates or functions using relatively intricate and sophisticated principles; examples include electronic equipment (camcorders, CD/DVD players, etc.), computers, fiber-optic systems, spacecraft, aircraft, and military rocketry.These advancedmaterials are typically traditional materials whose properties have been enhanced,and, also newly developed, high-performance materials. Furthermore, they may beof all material types (e.g., metals, ceramics, polymers), and are normally expensive.Advanced materials include semiconductors, biomaterials, and what we may term“materials of the future” (that is, smart materials and nanoengineered materials),which we discuss below. The properties and applications of a number of theseadvanced materials—for example, materials that are used for lasers, integratedcircuits, magnetic information storage, liquid crystal displays (LCDs), and fiberoptics

Phase diagram

A phase diagram- graphical representation of the combinations of temperature, pressure, composition, or other variables for which specific phases exist at equilibrium. For H_2O, a typical diagram shows the temperature and pressure at which ice (solid),water (liquid) and steam (gas) exist. Phase A phase diagrams show what phases exist at equilibrium and what phase transformations we can expect when we change one of the parameters of the system (T, P, composition).

Solid solutions

When homogeneous mixtures of 2 or more kinds of atoms occur in the solid state,they are known as solid solutions. The term solvent refers to the more abundant atomic form, and solute to the less abundant. Solid solutions occur in either of 2 distinct types. The first is known as a substitutional solid solution. In this case, a direct substitution of one type of atom for another occurs so that solute atoms enter the crystal to take positions normally occupied by solvent atoms. The other type of solid solution is shown in Fig. 9.1B. Here the solute atom (carbon)does not displace a solvent atom, but, rather, enters one of the holes, or interstics,between the solvent (iron) atoms. This type of solution is known as an interstitial solid solution.

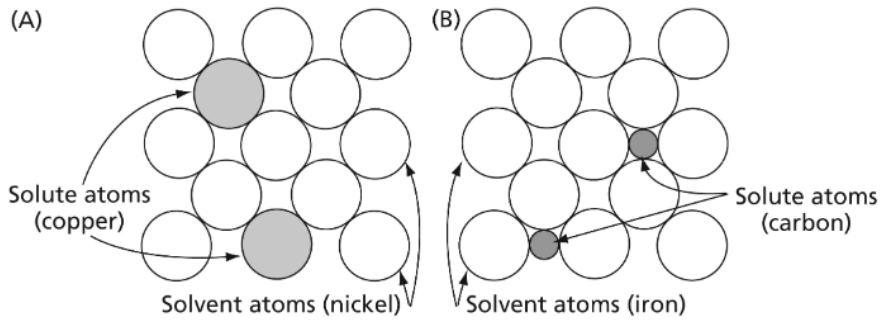


Fig The 2 basic forms of solid solutions.

a) In the interstitial example on the right, carbon is dissolved interstitially in the body-centered cubic form of iron.

b) For the substitutional solid solution shown on the left, the nickel atoms replace copper atoms.

Intermediate Phases

In many alloy systems, crystal structures or phases are found different from those of the elementary components (pure metals). These homogeneous crystal structures or phases are called intermediate phases. When the new crystal structures occur with simple whole-number fixed ratios of the component atoms, they are intermetallic compounds with stoichiometric compositions. The crystal structure with a composition at a ratio of approximately one zinc atom to one of copper is body-centered cubic. Because this body-centered cubic structure can exist over a range of compositions (it is the only stable phase at room temperature between 47 and 50 wt% of zinc), it is not a compound, but a solid solution. This is also sometimes called a nonstoichiometric compound or a nonstoichiometric intermetallic compound.**Fig** shows that solute atoms in interstitial alloys must be small in size. Extensive interstitial solid solutions occur only if the solute atom has an apparent diameter smaller than 0.59 that of the solvent. The 4 most important interstitial atoms are carbon, nitrogen, oxygen, and hydrogen, all of which are small in size. Small interstitial solute atoms dissolve much more readily in transition metals than in other metals. The ability of transition elements to dissolve interstitial atoms is believed to be due to their unusual electronic structure. All transition elements possess an incomplete electronic shell inside of the outer, or valence, electron shell. The no transition metals, on the other hand, have filled shells below the valence shell. The extent to which interstitial atoms can dissolve in the transition metals depends on the metal in question, but it is usually small.Interstitial atoms can diffuse easily through the lattice of the solvent. Diffusion occurs not by a vacancy mechanism, but by the solute atoms jumping from one interstitial position to another.

Solubility of carbon in body-centered cubic iron

The solubility of carbon in body-centered cubic iron is low. In fact, the number of carbon atoms in an iron crystal is roughly equivalent to the number of vacancies found in crystals.- The positions marked an x in Fig. 9.2 are those that carbon atoms take when they enter the iron lattice. They lie either midway between 2 corner atoms or in the centers of unit cell.- In the diamond lattice, the carbon atom has an apparent diameter of 0.1541 nm (Fig.9.2A). Fig. 9.2B shows that the lattice constant of iron is 0.2866 nm. The diameter of the iron atom is 0.2481 nm, and the width of the hole occupied by carbon atoms is only0.0385 nm. The lattice in the vicinity of each solute atom is badly strained, and work must be done in order to introduce the interstitial atom into the crystal.

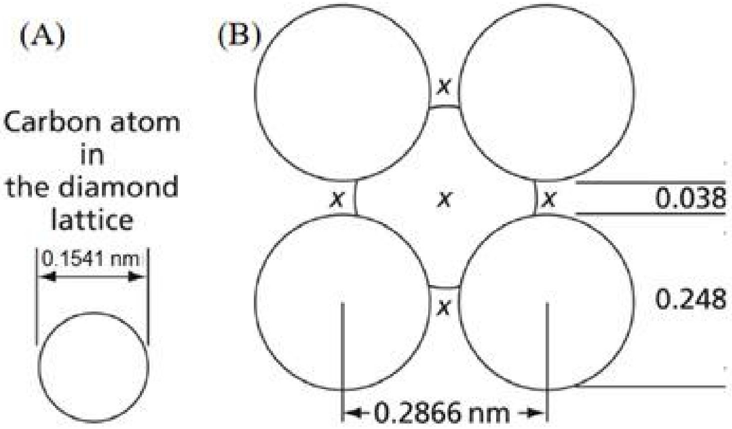


Fig. 9.2 The interstitial positions in the body-centered cubic iron unit cell that may be occupied by carbon atoms.

Fig. 9.3 shows a plot of the equilibrium carbon concentration between roomtemperature and 727°C (1000 K). The curve clearly shows that the solubility ofcarbon in ferrite is very small. The equilibrium value at room temperature is only8.5×10-12weight percent.At 727°C the carbon concentration reaches its maximum value, 0.022%.

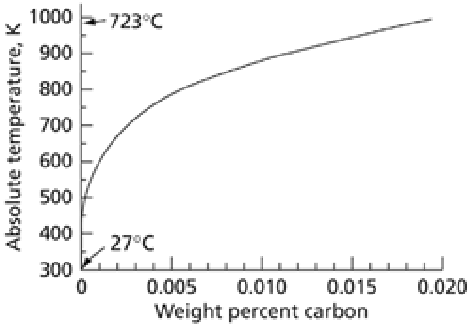


Fig. 9.3 Solubility of carbon in alpha-iron (body-centered cubic iron).

Hume-Rothery rule

Heterothermy pointed out that an extensive solid solubility of one metal in another only occurs if the diameters of the metals differ by less than 15%. This criterion for solubility is known as the size factor and is directly related to the strains produced in the lattice of the solvent by the solute atoms.One of the most important requirements is the relative positions in the electromotive series. When metals lie close to each other in the electromotive series, they tend to act as if they were chemically the same, which leads to metallic bonding instead of ionic.Two other factors are of importance, especially when one considers a completely soluble system. Even if the size factor and electromotive series positions are favorable, such a system is only possible when both components (pure metals) have the same valence, and crystallize in the same lattice form.

1.Size factor:

the atomic diameter should be compatible between solute atoms and solvent atoms. The difference of the atomic diameter between solute atoms and solvent atoms should be not more than 15%.Cu (2.55 A)-Zn (2.65 A) difference= 4%--soluble (2.55 A)-Cd(2.97 A) difference=16.5%insolubleGreatCdatomic size—great lattice distortion—Cu-Cdsystem spontaneously or preferably forCuCdcompound in Cu matrix

2.Electrochemical factor:

Although the atomic diameters may be favorable, solid solutions will not form when there is a strong chemical tendency for A and B to form “intermetallic compound “A is strong electropositive (e.g., Na, as compared to Cl)B is strong electronegative (e.g., Cl, as compared to Na)** Na, Cl-ionic compound, instead of solution** Cu (more electropositive)–As (more electronegative)

2.Relative valence factor:

Metal of low valence is more likely to dissolve the metal which has high valencee.g., Zn (+2) dissolved easily in Cu (+1)But Cu is not likely dissolved in ZnCompletely soluble: same valence and same lattice structuree.g. Cu-Ni system

Gibb’s Phase rule:

It was stated by Williams Gibbs in 1874. It may be stated as, *“When an equilibrium between any number of phases is influenced only by temperature, pressure and concentration, but not influenced by gravity, or electrical or magnetic forces or by surface tension then the number of degree of freedom (F) of the system is related to the number of components (C) and of phases (P) by the phase rule equation”.*

The mathematical representation of phase rule is **F = C – P + 2.**

Advantages:

1. It is applicable to both chemical and physical equilibria.
2. It is applicable to macroscopic systems and hence no information is required regarding molecular, micro structure.
3. We can conveniently classify equilibrium states in terms of phases, components and degree of freedom.
4. The behaviour of system can be predicted under different conditions.
5. According to phase rule, different systems behave similarly if they have same degrees of freedom.
6. Phase rule helps in deciding under a given set of conditions:

   (a) Existence of equilibrium among various substances.

   (b) Inter convergence of substances.

   (c) Disappearance of some of the substances.

Limitations:

1. It is applicable only for the systems which are in equilibrium.
2. Only three degrees of freedom Viz., Temperature, pressure and composition are allowed to influence the equilibrium systems.
3. Under the same conditions of temperature and pressure, all the phases of the system must be present.
4. It considers only the number of phases, rather than their amounts.

Phase diagram: The diagram which represents the conditions of equilibrium between different phases is called phase diagram.

One component system: The water system consists of 3 phases, viz., ice, water & water vapour.

$$\text{Ice}_{(s)} \leftrightarrow \text{Water}_{(l)} \leftrightarrow \text{Water vapour}_{(g)}$$

Water is the only chemical compound involved; hence the number of components is one

(C = 1). From phase rule, $F = C – P + 2 = 1 – P + 2 = 3 – P$

i.e. the degree of freedom depends on the number of phases present at equilibrium. Three different cases are possible.

(a) P = 1, F = 2 (Bivariant system)

(b) P = 2, F = 1 (Univariant system)

(c) P = 3, F = 0 (Invariant system)

Condensed phase rule / reduced phase rule: The phase rule equation is $F = C – P + 2$.

For a two component system, C = 2 then $F = 2 – P + 2 = 4 – P$

The minimum number of phase at equilibrium is one. Then $F = 4 – 1 = 3$.

Hence the maximum number of degree of freedom is three and temperature, pressure and composition are required to define the system. This leads to 3 dimensional figures which cannot be explained on a paper. Hence one of the three variable to be kept constant.

$F = C – P + 1$ (Two component system)

$F = 2 – P + 1 = 3 – P$. This is the reduced / condensed form of the phase rule.

Thermal analysis:“*Thermal analysis is the study of the cooling curves of various compositions of a system during solidification*”. It is used for finding the shape of the freezing – point curves of any system especially those involving metals. For any mixture of a definite composition, it is possible to find out freezing point and eutectic point from the cooling curves.

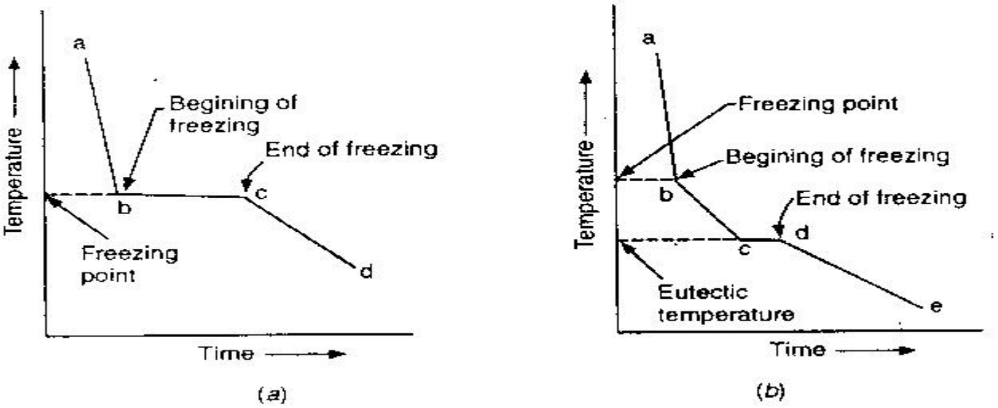


Figure: (a). When a pure substance in the fused state is allowed to cool slowly & the temperature noted at definite intervals. The graph of rate of cooling will be continuous curve. When the freezing point is reached and the solid makes its appearances by the break in the continuity of the cooling curve and the temperature remains constant, until the liquid is fully solidified. There after, the fall in temperature will again become continuous.

Figure: (b). When a mixture of two solids in the fused state is allowed to cool slowly & the temperature noted at definite intervals. The graph of rate of cooling will be continuous curve. When a solid phase begins to form, the rate of cooling curve exhibits a break. However, the temperature does not remain constant as in the previous case of cooling of a pure substance. The temperature decreases continuously until the eutectic point reached. Now the temperature remains constant, till the completion of solidification. There after, the fall of temperature becomes uniform, but the rate of fall is quite different from the previous one.

Applications:

1. The melting point and eutectic temperature of various solids can be obtained.
2. The percentage of the compounds can be found out.
3. The behaviour of the compound can be understood from the cooling curve.
4. The procedure of thermal analysis can be used to derive the phase diagram of any two component system.

<u>Eutectic system:</u>Eutectic – Easy to melt. Consider a binary system in which two components are miscible in all proportions in the liquid (molten) state. They do not react chemically and each component has the property of lowering each other's freezing point. Such a binary system is called Eutectic system.

Eutectic mixture: "*A solid solution of two component system which has the lowest freezing point of all the possible mixtures of the components is called eutectic mixture*".

Eutectic point:*Minimum freezing point attainable corresponding to the eutectic mixture is called eutectic point (means lowest melting point).* The eutectic mixture has a definite composition and a sharp melting point. In this respect it resembles a compound. However, it is not a compound for the components are not present in stoichiometric proportions. When the solid was examined under a powerful microscope, both the constituents were seen to lie as separate crystals. Moreover, physical properties such as density and heat of solution of eutectic solid were almost equal to the mean values of the constituents. Hence it is a mixture and not a chemical compound.

Applications:

1. Alloys which are known to form eutectic mixture's are used as 'fail – safe' device in boilers, as plugs in automobiles, fire – splinklers and other such safety devices.
2. Eutectic systems, because of their low melting points are also used for joining two metal pieces together. Example: Pb – Sn solders.

Lead – Silver system: It is a two – component system with four possible phases – solid Ag, solid Pb, solution of Ag + Pb and its vapour. The two metals are completely miscible with each other in liquid state and do not form any chemical compound. There is almost no effect of pressure on equilibrium, the temperature and composition are considered to construct the phase diagram at constant atmospheric pressure.

It consists of (1) Curves AO and BO.

(2) Eutectic point – "O" .

(3) Areas: Above AOB / Below AO / Below BO.

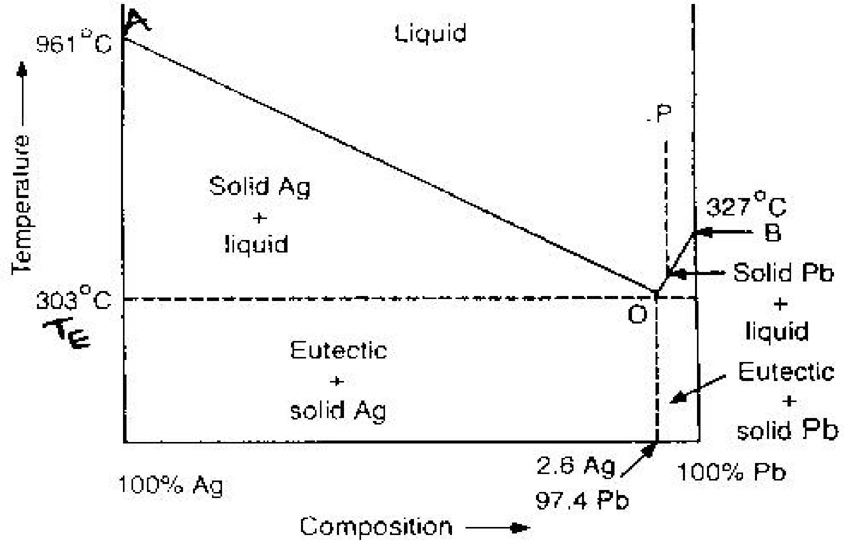
Curves AO & BO:

CURVE AO	CURVE BO
It is the freezing point curve of Ag (961^{o}C)	It is the freezing point curve of Pb (327^{o}C)
It shows decrease in freezing point / melting point of Ag due to the addition of Pb to Ag	It shows decrease in freezing point / melting point of Pb due to the addition of Ag to Pb.
Solid Ag is equilibrium with solution of Pb in Ag.	Solid Pb is equilibrium with solution of Ag in Pb.

Here C = 2 and P = 2, then the reduced phase rule is F = C – P + 1 = 2 – 2 +1 = 1.

Hence the system is univariant. The point O (303^{o}C) represents a fixed composition of 97.4 % Pb and 2.6 % Ag, and is called eutectic composition. On cooling, the whole mass crystallizes out as such.

Eutectic point 'O': The curves AO & BO meet at the point O is called eutectic point. Here, solid Ag, Solid Pb and solution of Ag & Pb are in equilibrium. Thus, C = 2 & P = 3. Hence the reduced phase rule is F = C – P + 1 = 2 – 3 + 1 = 0 and the system is invariant.



The point 'O' (303^{o}C) represents a fixed composition of 97.4 % Pb and 2.6 % Ag, and is called eutectic composition.

Area above AOB: The components Ag & Pb are exist as solution. Thus, C = 2 & P = 1.

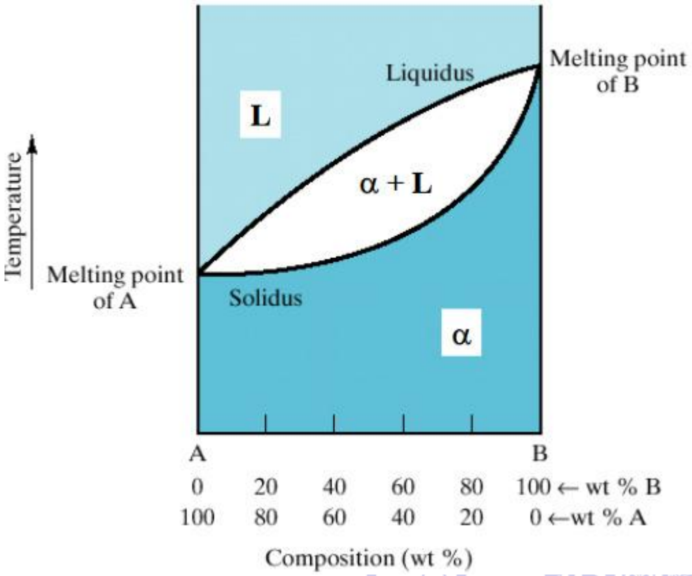
Hence f = C – P + 1 = 2 – 1 + 1 = 2, the system is bivariant. The system will exist when the temperature T > 303^{o}C , Pb < 97.4 % and Ag > 2.6 %.

AREA	EXISTENCE	P	C	F
Below AO	Ag + Solution of Pb / Ag	2	2	1
Below BO	Pb + solution of Ag / Pb	2	2	1
Below T_E line	Solid Ag + Solid Pb	2	2	1

All these areas have P = 2 and F = 1. The system is univariant.

Binary Isomorphous Systems (I)

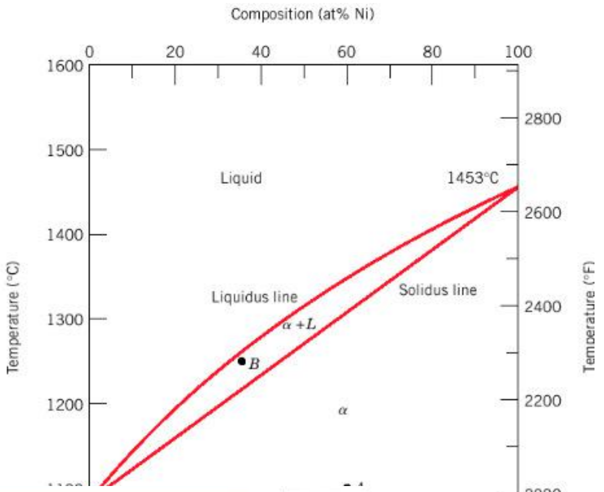
Isomorphous system-complete solid solubility of the two components (both in the liquid and solid phases).



Three phase region can be identified on the phase diagram: Liquid (L) , solid + liquid (α +L), solid (α)Liquidus line separates liquid from liquid + solidSolidusline separates solid from liquid + solid.

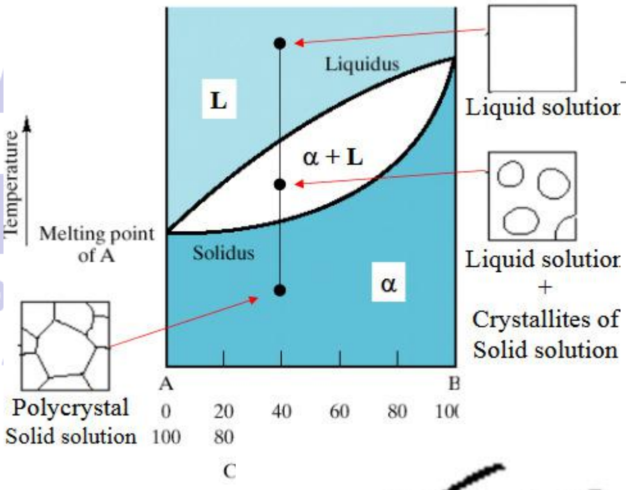
Example of isomorphous system: Cu-Ni(the complete solubility occurs because both Cu and Ni have the same crystal structure, FCC, similar radii, electronegativity and valence).

In one-component system melting occurs at a well-defined melting temperature.In multi-component systems melting occurs over the range of temperatures, between the solidus and liquidus lines. Solid and liquid phases are in equilibrium in this temperature range.



Interpretation of Phase Diagrams

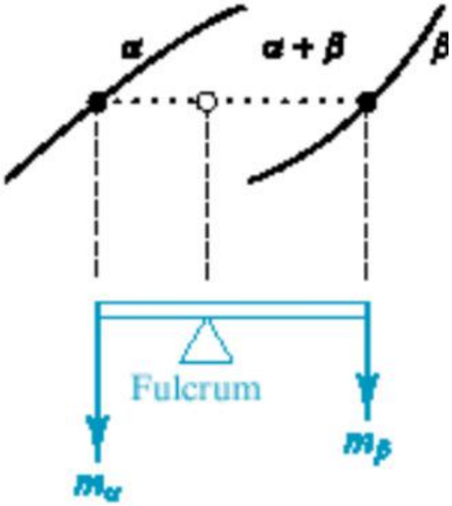
For a given temperature and composition we can use phase diagram to determine:1) The phases that are present2) Compositions of the phases3) The relative fractions of the phasesFinding the composition in a two-phase region:1. Locate composition and temperature in diagram 2. In two phase regions draw the tie lineor isotherm 3. Note intersection with phase boundaries. Read compositions at the intersections. The liquid and solid phases have these compositions.



The Lever Rule

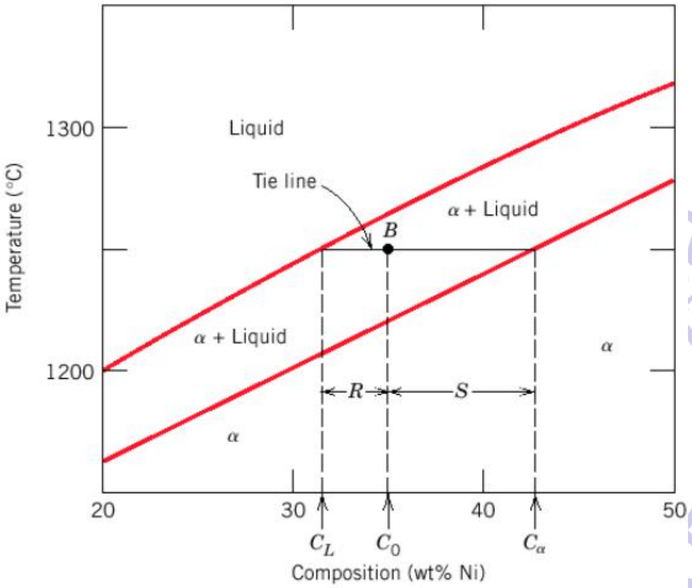
Finding the amounts of phases in a two-phase region:

1. Locate composition and temperature in diagram



2. In two phase regions draw the tie line or isotherm

3. Fraction of a phase is determined by taking the length of the tie line to the phase boundary for the other phase, and dividing by the total length of tie line.



The lever rule is a mechanical analogy to the mass balance calculation. The tie line in the two-phase region is analogous to a lever balanced on a fulcrum.

Mass fractions: $W_L = S / (R+S) = (C_\alpha - C_o) / (C_\alpha - C_L)$

$W_\alpha = R / (R+S) = (C_o - C_L) / (C_\alpha - C_L)$

Derivation of the lever rule

$W_L = (C_\alpha - C_o) / (C_\alpha - C_L)$

1)All material must be in one phase or the other:

$$W_\alpha + W_L = 1$$

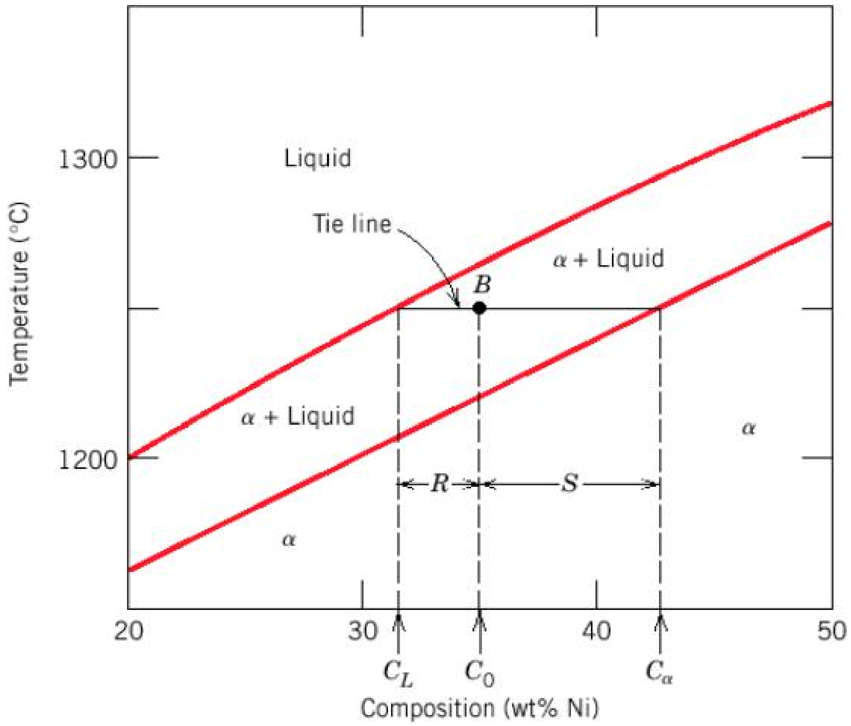
2) Mass of a component that is present in both phases equal to the mass of the component in one phase + mass of the component in the second phase:

$$W_\alpha C_\alpha + W_L C_L = C_o$$

3) Solution of these equations gives us the Lever rule.

$$W_\alpha = (C_o - C_L) / (C_\alpha - C_L)$$

Phase compositions and amounts. An example.



C_o= 35 wt. %, C_L= 31.5 wt. %, C_α= 42.5 wt. %

Mass fractions:

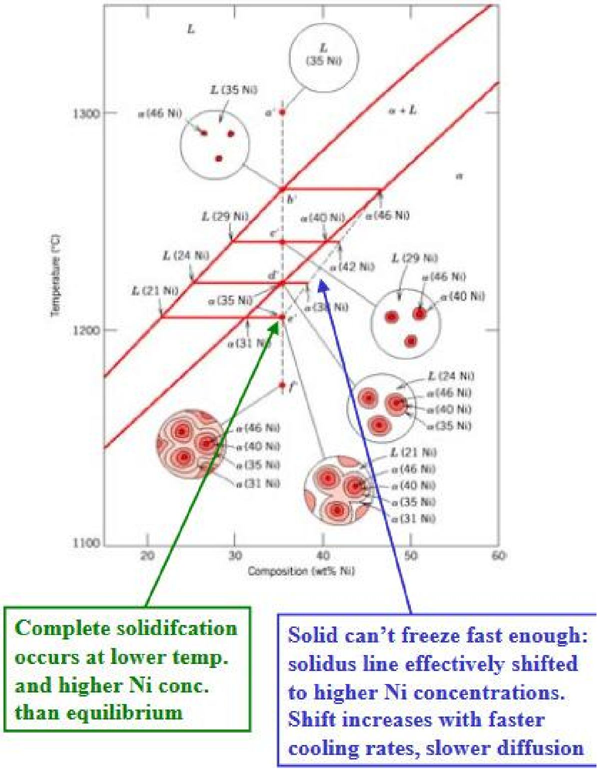
$W_L = (C_\alpha - C_o) / (C_\alpha - C_L) = 0.68$

$W_\alpha = (C_o - C_L) / (C_\alpha - C_L) = 0.32$

Development of microstructure in isomorphous alloys

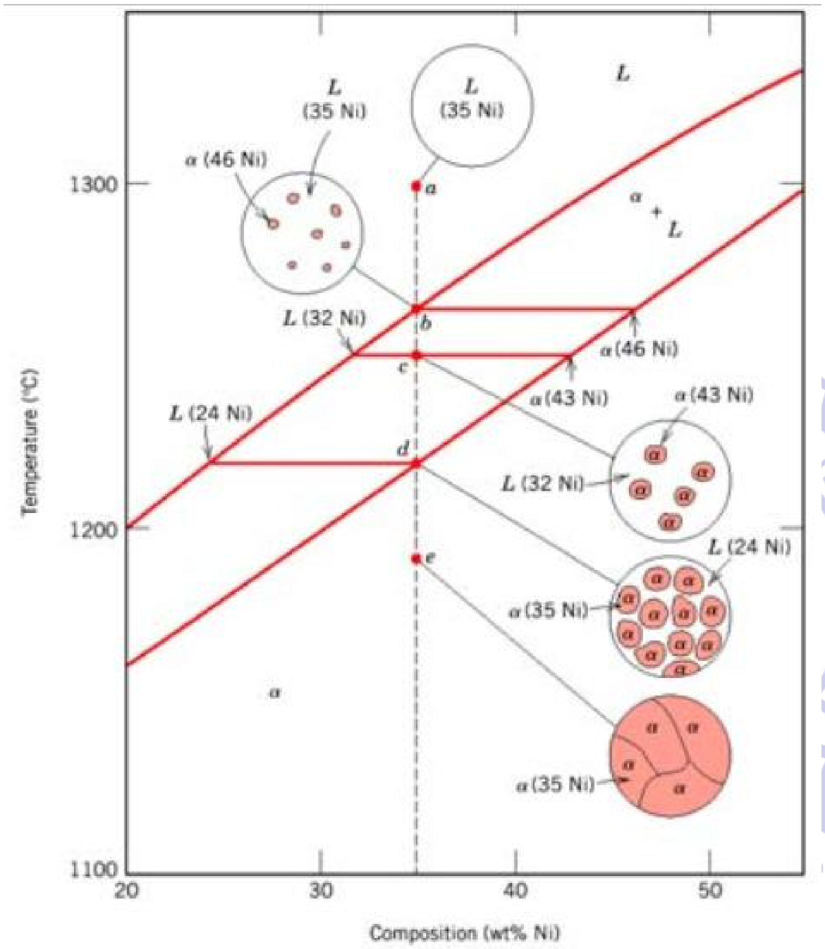
Equilibrium (very slow) cooling

- Solidification in the solid + liquid phase occurs gradually upon cooling from the liquidus line.
- The composition of the solid and the liquid change gradually during cooling (as can be determined by the tie-line method.)
- Nuclei of the solid phase form and they grow to consume all the liquid at the solidus line.



Complete solidifcation occurs at lower temp. and higher Ni conc. than equilibrium

Solid can't freeze fast enough: solidus line effectively shifted to higher Ni concentrations. Shift increases with faster cooling rates, slower diffusion



Compositional changes require diffusion in solid and liquid phases

- Diffusion in the solid state is very slow. ⇒The new layers that solidify on top of the existing grains have the equilibrium composition at that temperature but once they are solid their composition does not change. ⇒Formation of layered (cored) grains and the invalidity of the tie-line method to determine the composition of the solid phase.

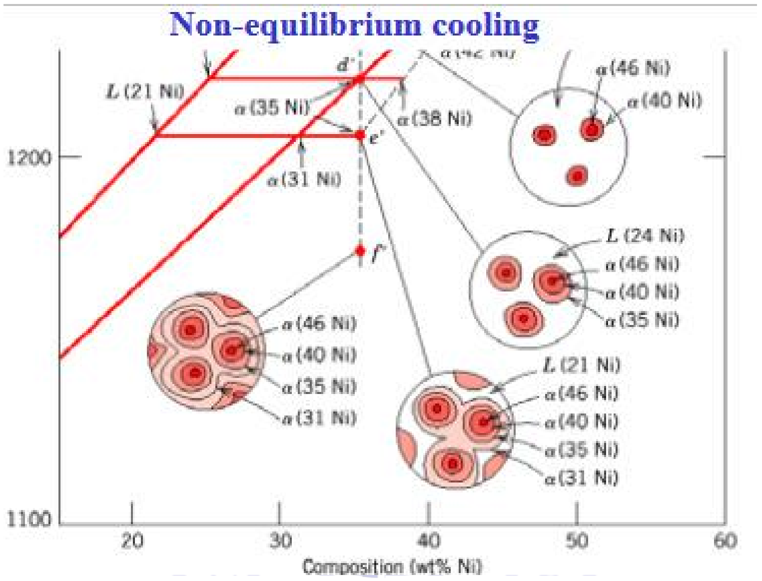
- The tie-line method still works for the liquid phase, where diffusion is fast. Average Ni content of solid grains is higher. ⇒Application of the lever rule gives us a greater proportion of liquid phase as compared to the one for equilibrium cooling at the same T. ⇒Solidus line is shifted to the right (higher Ni contents), solidification is complete at lower T, the outer part of the grains are richer in the low-melting component (Cu).

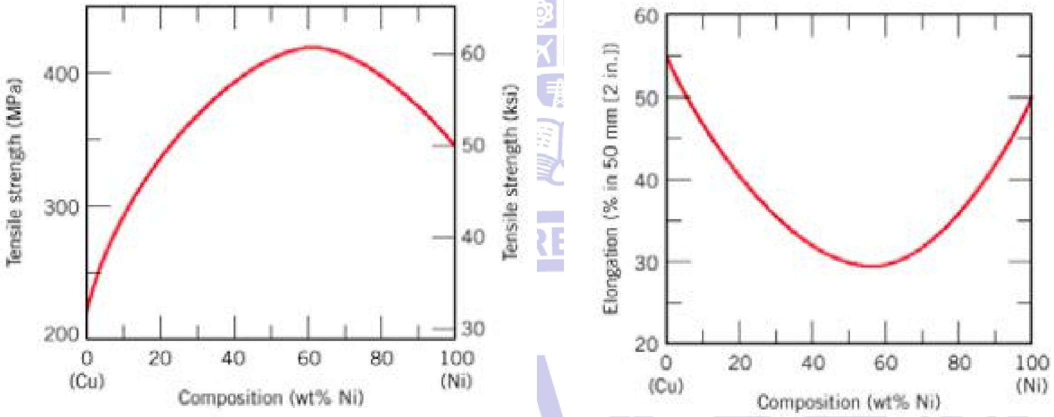
- Upon heating grain boundaries will melt first. This can lead to premature mechanical failure.

Note that the center of each grain is rich in higher mp constituent (freezes first), with compositional gradient to edge of grain: segregation

•The resulting microstructure is termed a cored structure

•On re-heating, GBs will melt first, as they are rich in lower mp constituent. This can lead to premature mechanical failure!





Mechanical properties of isomorphous alloysSolid solution strengthening

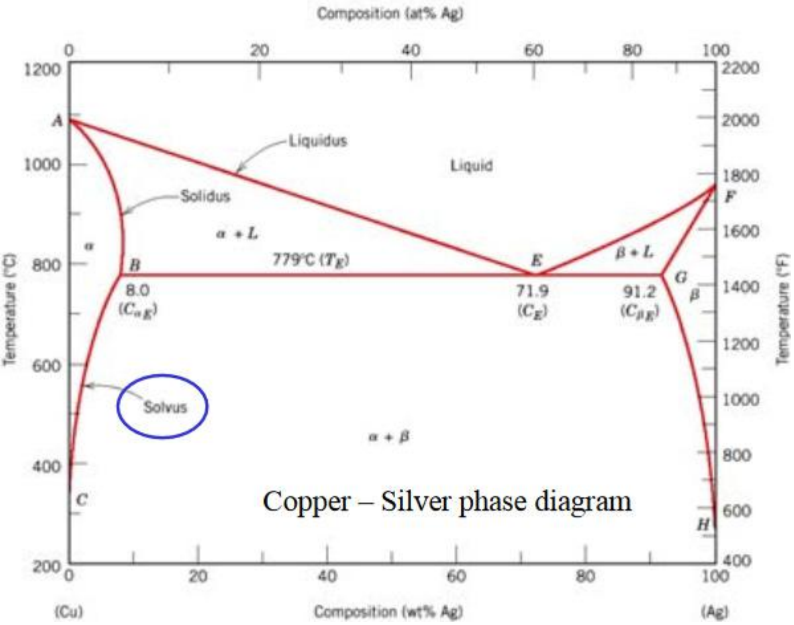
Binary Eutectic Systems

- Three single phase regions (α- solid solution of Ag in Cu matrix, β= solid solution of Cu in Ag marix, L - liquid)

- Three two-phase regions

(α+ L, β+L, α+β)

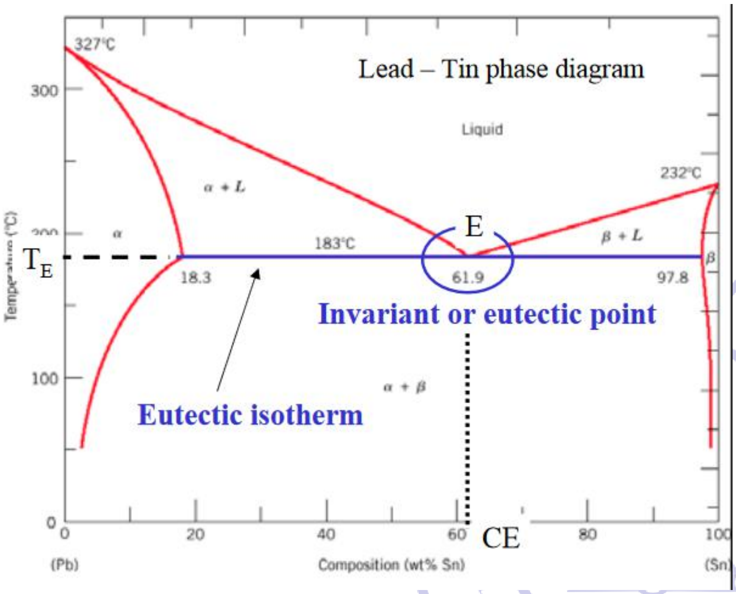
- Solvus line separates one solid solution from a mixture of solid solutions. The Solvus line shows limit of solubility



Copper – Silver phase diagram

Eutectic or invariant point- Liquid and two solid phases co-exist in equilibrium at the eutectic composition C_E and the eutectic temperature T_E.

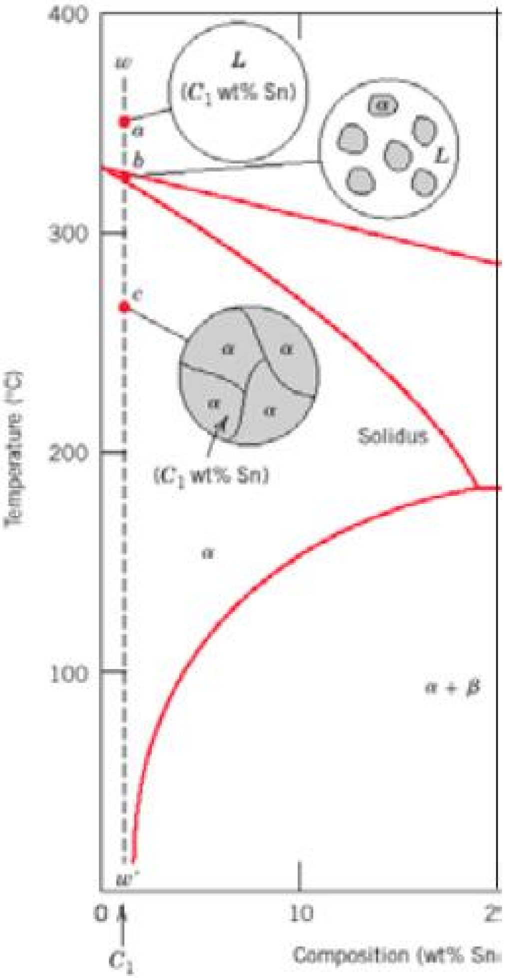
Eutectic isotherm- the horizontal solidus line at T_E.



General Rules: Eutectic reaction– transition between liquid and mixture of two solid phases, α+ βat eutectic concentration C_E. The melting point of the eutectic alloy is lower than that of the components (eutectic = easy to melt in Greek). At most two phases can be in equilibrium within a phase field. Three phases (L, α, β) may be in equilibrium only at a few points along the eutectic isotherm. Single-phase regions are separated by 2-phase regions.

Development of microstructure in eutectic alloys:

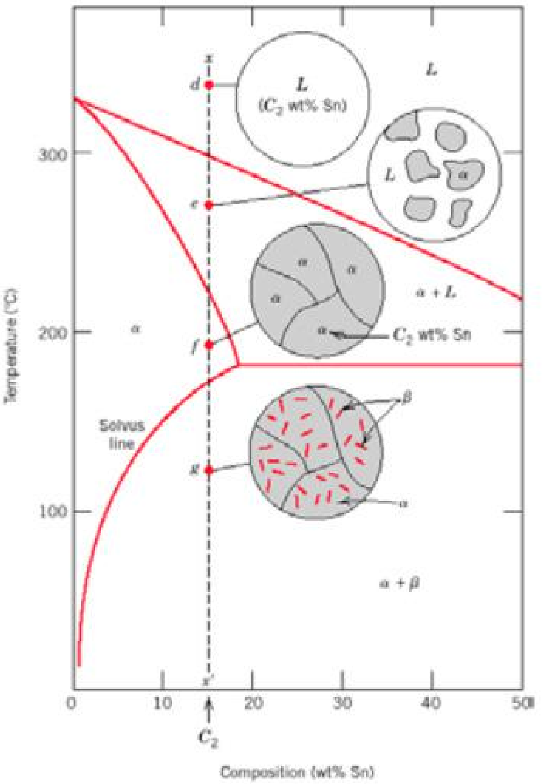
Several different types of microstructure can be formed in slow cooling adifferent composition. Let's consider cooling of liquid lead – tin system at different compositions.

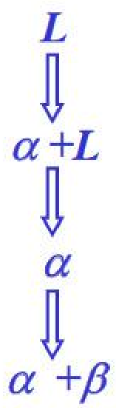


In this case of lead-rich alloy (0-2 wt. % of tin) solidification proceeds in the same manner as for isomorphous alloys (e.g. Cu-Ni) that we discussed earlier.

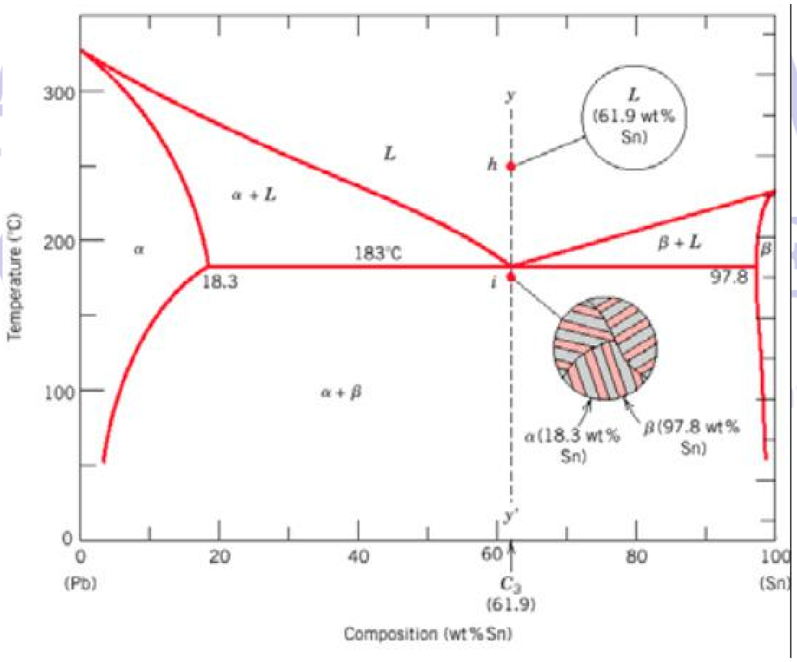
$$L \rightarrow \alpha + L \rightarrow \alpha$$

At compositions between the room temperature solubility limit and the maximum solid solubility at the eutectic temperature, βphase nucleates as the αsolid solubility is exceeded upon crossing the solvus line.



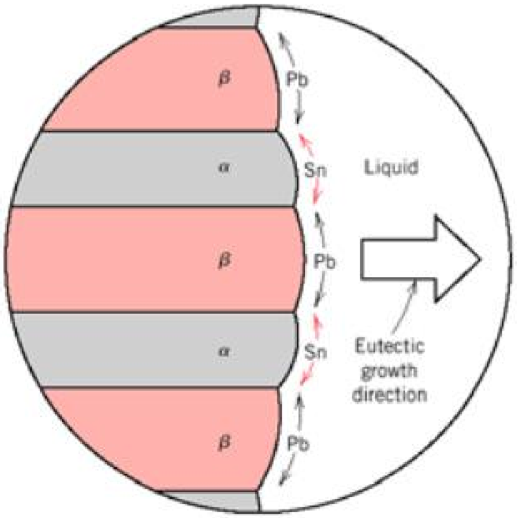


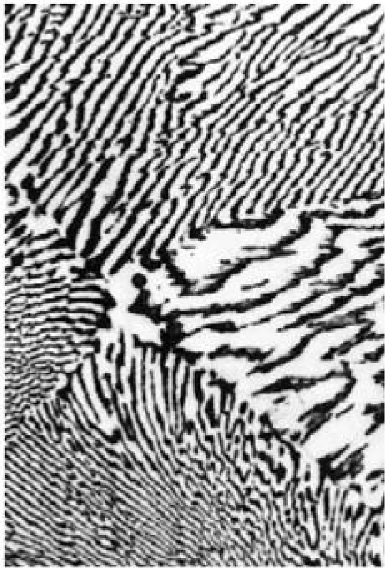
No changes above the eutectic temperature TE. At TEthe liquid transforms to αand βphases (eutectic reaction).



L→α+β

Solidification at the eutectic composition (II)Compositions of αand βphases are very different →the eutectic reaction involves redistribution of Pb and Sn atoms by atomic diffusion. This simultaneous formation of αand βphases result in a layered (lamellar) microstructure that is called the eutectic structure.

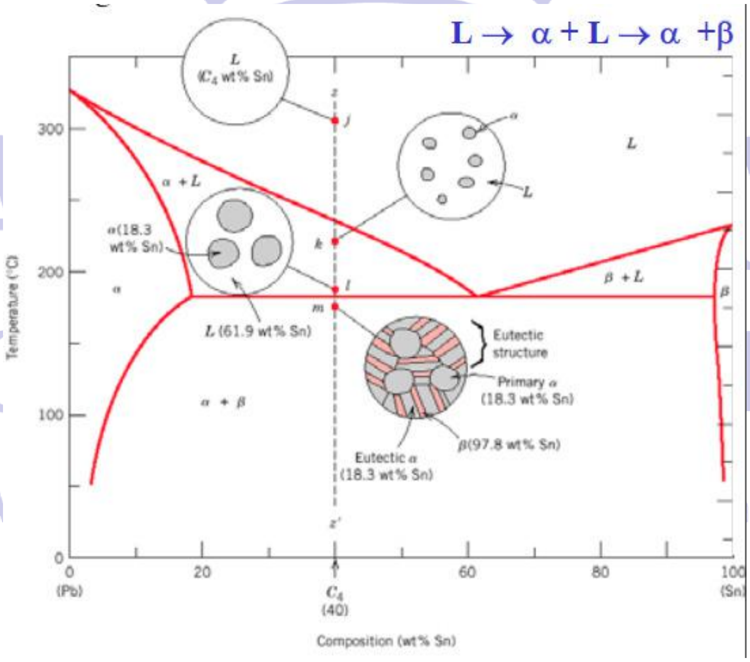




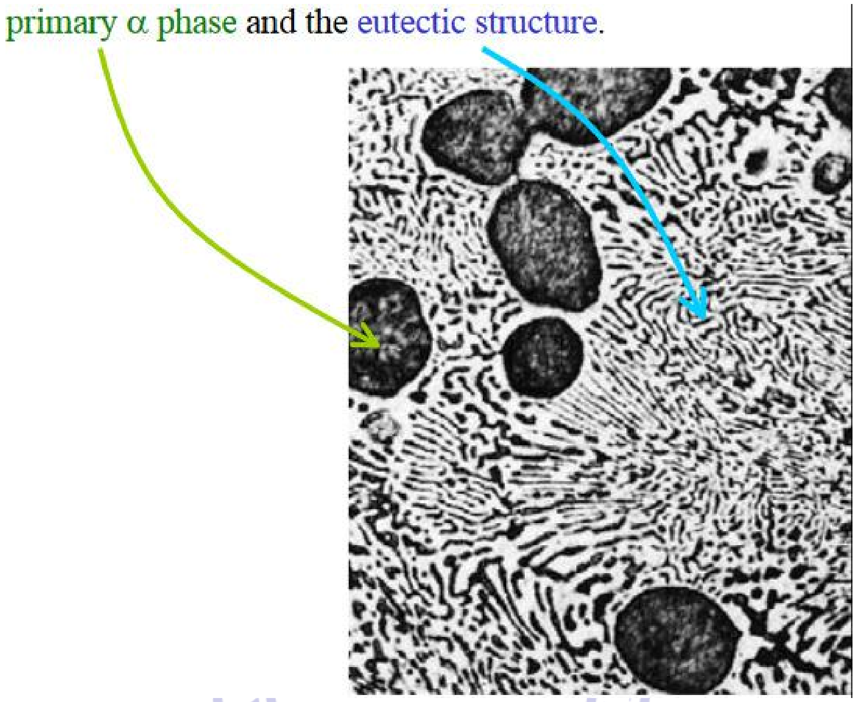
Formation of the eutectic structure in the lead-tin system.In the micrograph, the dark layers are lead-reach αphase, the light layers are the tin-reach βphase.

Compositions other than eutectic but within the range of the eutectic isotherm

Primary αphase is formed in the α+ L region, and the eutectic structure that includes layers of αand βphases (called eutectic αand eutectic βphases) is formed upon crossing the eutectic isotherm.



Microconstituent –element of the microstructure having a distinctive structure. In the case described in the previous page, microstructure consists of two microconstituents, primary αphaseand the eutectic structure.



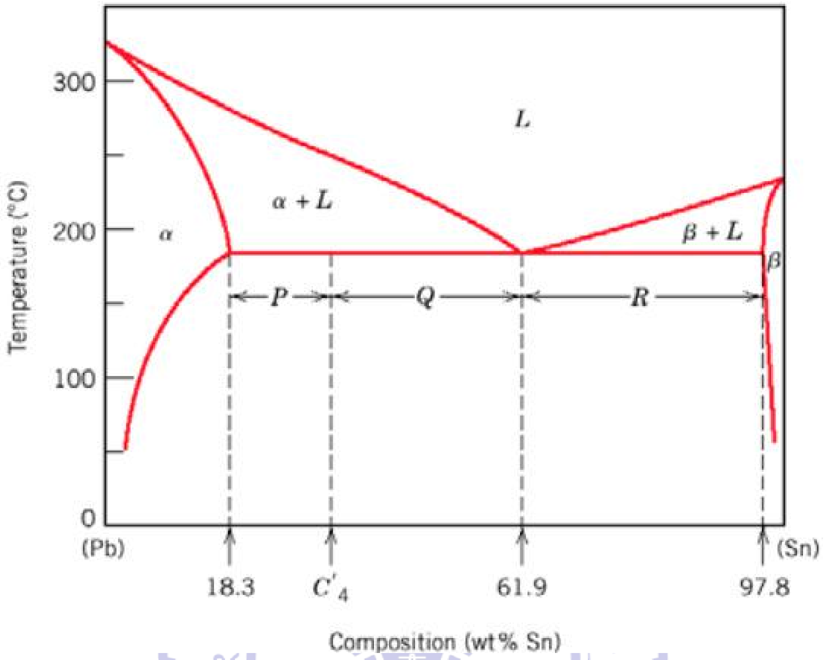
Although the eutectic structure consists of two phases, it is a microconstituent with distinct lamellar structure and fixed ratio of the two phases.

How to calculate relative amounts of microconstituents?

Eutectic microconstituent forms from liquid having eutectic composition (61.9 wt% Sn)

We can treat the eutectic as a separate phase and apply the lever rule to find the relative fractions of primary αphase (18.3 wt% Sn) and the eutectic structure (61.9 wt% Sn):

We= P / (P+Q)(eutectic) Wα’= Q / (P+Q)(primary)



How to calculate the total amount of αphase (both eutectic and primary)?

Fraction of αphase determined by application of the lever rule across the entire α+ βphase field:

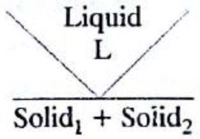
W_{α}= (Q+R) / (P+Q+R) (αphase)

W_{β}= P / (P+Q+R) (βphase)

Eutectic

- In an eutectic reaction, when a liquid solution of fixed composi-tion, solidifies at a constant temperature, forms a mixture of two or more solid phases without an intermediate pasty stage. This process reverses on heating.

$$\text{Liquid} \underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}} \text{Solid}_1 + \text{Solid}_2$$

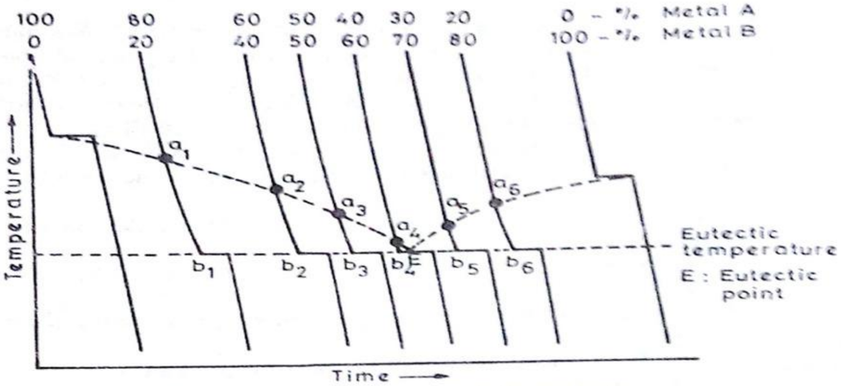


- In eutectic system, there is always a specific alloy, known as eutectic composition, that freezes at a lower temp. than all other compositions.
- At the eutectic temp. two solids form simultaneously form a single liquid phase.
- The eutectic temp. & composition determine a point on the phase dia, called the eutectic point.

Binary alloy eutectic system can be classed as:

1. One in which, two metals are completely soluble in the liquid state but are insoluble in each other in the solid state.

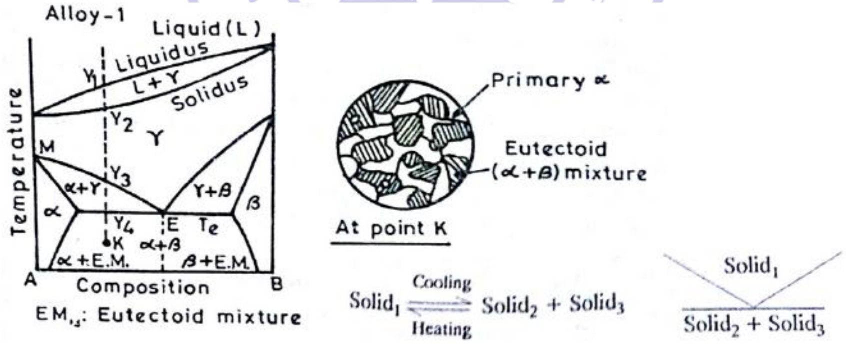
2. two metals are completely soluble in the liquid state but are partly soluble in each other in the solid state.



Cooling curves for two metals insoluble in solid state.

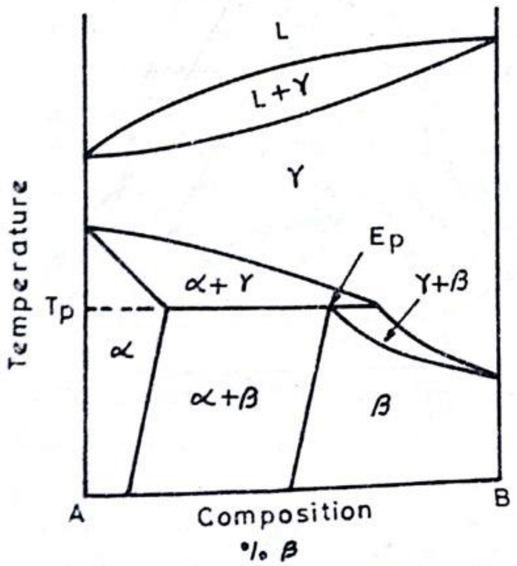
Eutectoid Transformation:

- Eutectoid reaction is an isothermal reversible reaction in which a solid phase (usually solid solution) is converted into two or more intimately mixed solids on cooling, the number of solids formed being the same as the number of component in the system.



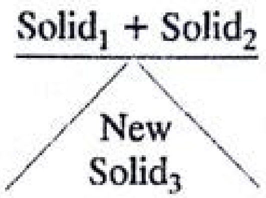
An eutectoid diagram.

The peritectoid reaction is the transformation of two solid into a third solid.

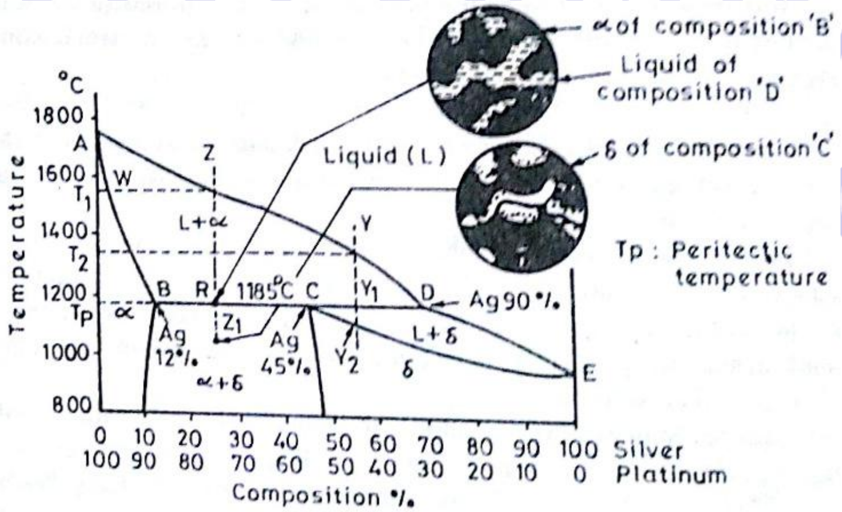


A peritectoid diagram.

$$\text{Solid}_1 + \text{Solid}_2 \underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}} \text{New Solid}_3$$

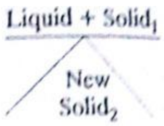


- Peritectic reaction:



Peritectic Reaction (Platinum-Silver Equilibrium Diagram).

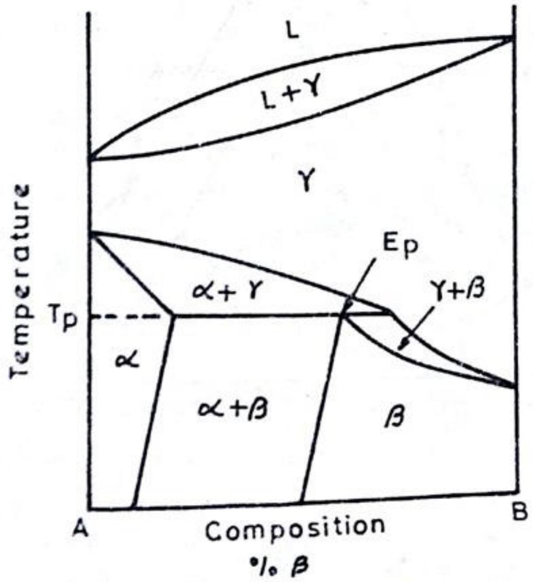
$$\text{Liquid} + \text{Solid}_1 \underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}} \text{New Solid}_2$$



- It is the reaction that occurs during the solidification of some alloys where the liquid phase reacts with a solid phase to give a solid phase of different structure.
- Assuming very slow rates of cooling, the peritectic reaction will occur only in those Pt-Ag alloys that Contain between 12 and 69% silver (Ag).
- Consider a liquid (melt) of composition Z, i.e., containing 25% Ag. Solidification commences at T1 and dendrites of α, initially of composition W, begin forming.
- Selective crystallization of α continues down to Tp, the peritectic temperature; when the alloy reaches. this temperature, it is composed of solid α-dendrites of composition B and liquid of composition D in the proportion α : liquid = RD : RB.

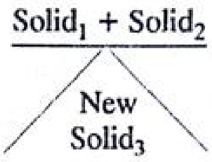
Peritectoid Transformation:

The peritectoid reaction is the transformation of two solid into a third solid.



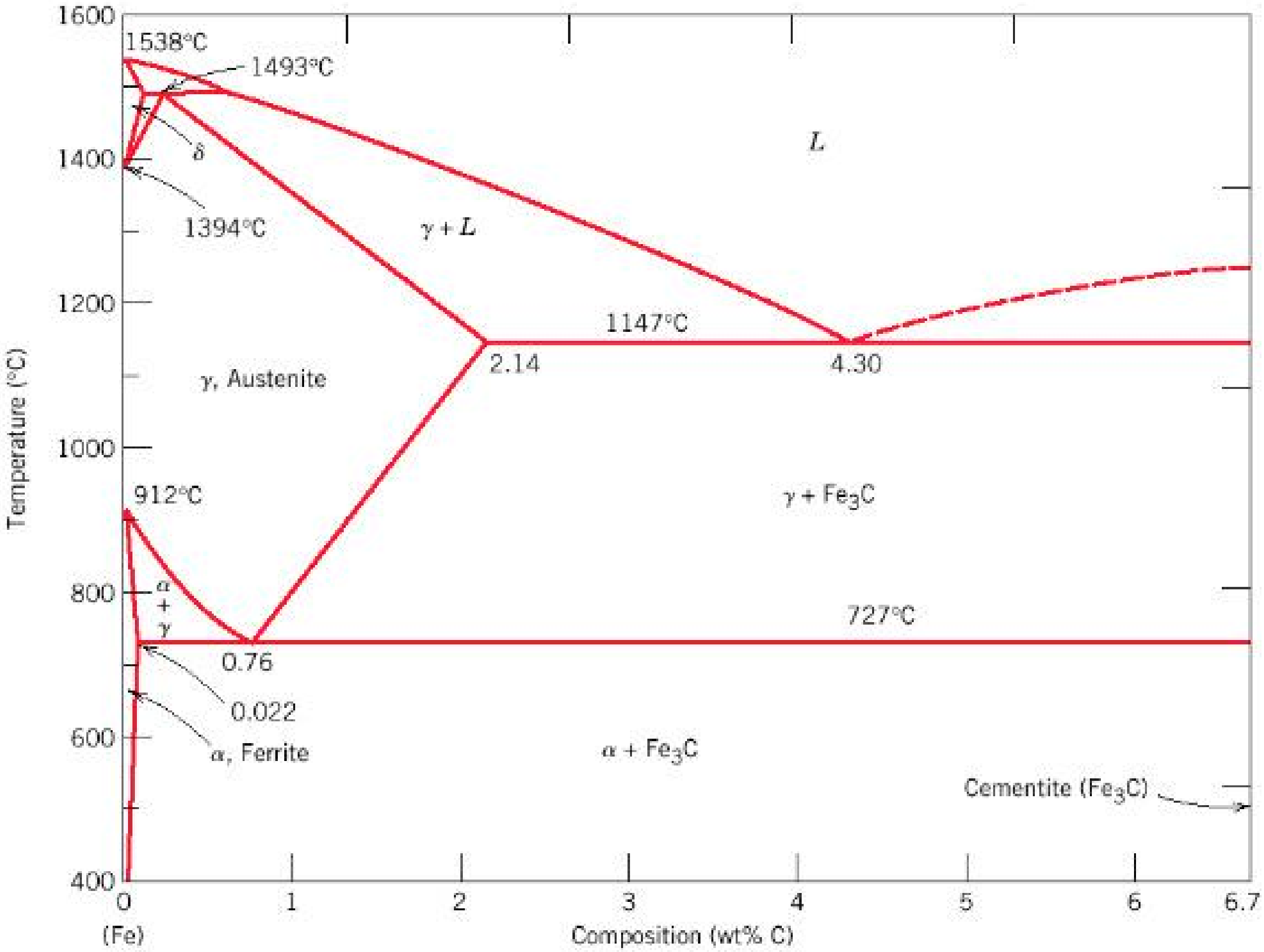
A peritectoid diagram.

$$\text{Solid}_1 + \text{Solid}_2 \underset{\text{Heating}}{\overset{\text{Cooling}}{\rightleftharpoons}} \text{New Solid}_3$$



The Iron–Iron Carbide (Fe–Fe3C) 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 part of the diagram, up to around 7% Carbon.



Phases in Fe–Fe_3C Phase Diagram

- α-ferrite - solid solution of C in BCC Fe
  - Stable form of iron at room temperature.
  - The maximum solubility of C is 0.022 wt%
  - Transforms to FCC γ-austenite at 912 °C
- γ-austenite - solid solution of C in FCC Fe
  - The maximum solubility of C is 2.14 wt %.
  - Transforms to BCC δ-ferrite at 1395 °C
  - Is not stable below the eutectic temperature (727 °C) unless cooled rapidly (Chapter 10)
- δ-ferrite solid solution of C in BCC Fe
  - The same structure as α-ferrite
  - Stable only at high T, above 1394 °C

• Melts at 1538 °C¾Fe3C (iron carbide or cementite)

• This intermetallic compound is metastable, it remains as a compound indefinitely at room T, but decomposes (very slowly, within several years)into α-Fe and C (graphite) at 650 - 700 °C

- Fe-C liquid solution

C is an interstitial impurity in Fe. It forms a solid solution with α, γ, δ phases of iron

Maximum solubility in BCC α-ferrite is limited (max. 0.022 wt% at 727 °C) - BCC has relatively small interstitial positions

Maximum solubility in FCC austenite is 2.14 wt% at 1147 °C - FCC has larger interstitial positions

Mechanical properties: Cementite is very hard and brittle -can strengthen steels. Mechanical properties also depend on the microstructure, that is, how ferrite and cementite are mixed.

Magnetic properties: α-ferrite is magnetic below 768 °C, austenite is non-magnetic

Classification. Three types of ferrous alloys:

•Iron: less than 0.008 wt % C in α–ferrite at room T

•Steels: 0.008 - 2.14 wt % C (usually < 1 wt%) α-ferrite + Fe3C at room T (Chapter 12)

•Cast iron: 2.14 - 6.7 wt % (usually < 4.5 wt %)

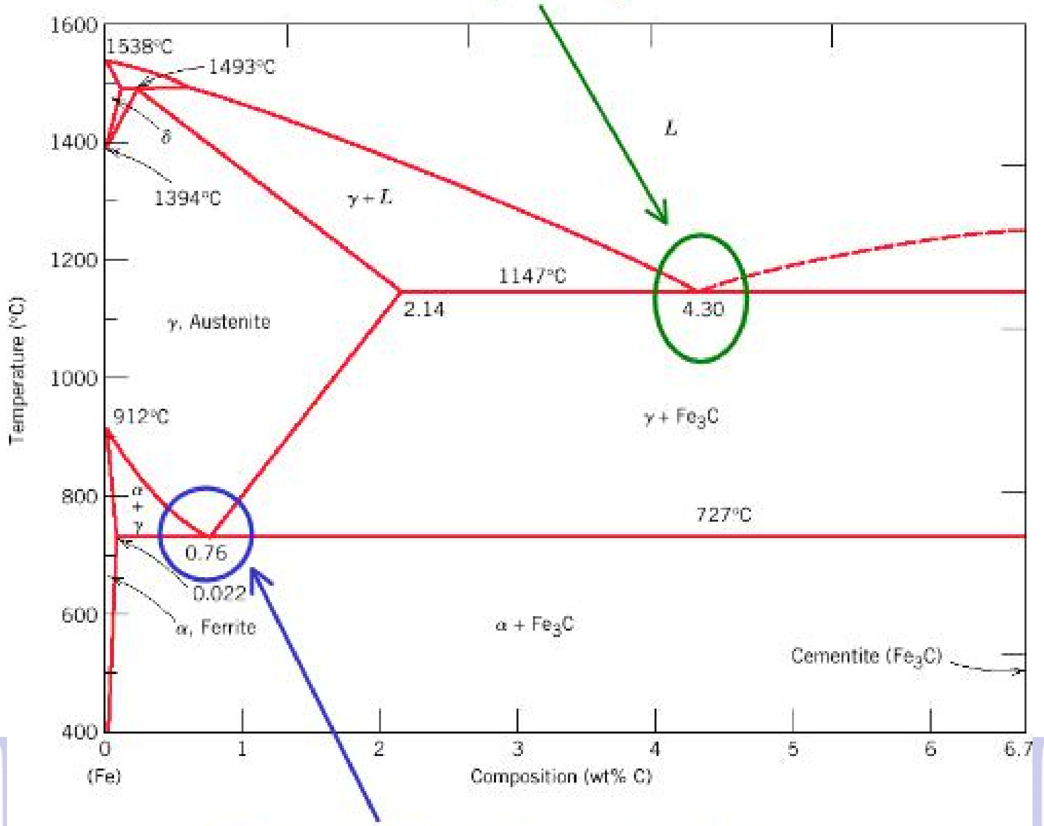
Eutectic and eutectoid reactions in Fe–Fe3C

Eutectoid: 0.76 wt%C, 727 °Cγ(0.76 wt% C) ↔α(0.022 wt% C) + Fe3C

Eutectic and eutectoid reactions in Fe–Fe_3C

Eutectic: 4.30 wt% C, 1147 °C

$$L \leftrightarrow \gamma + Fe_3C$$

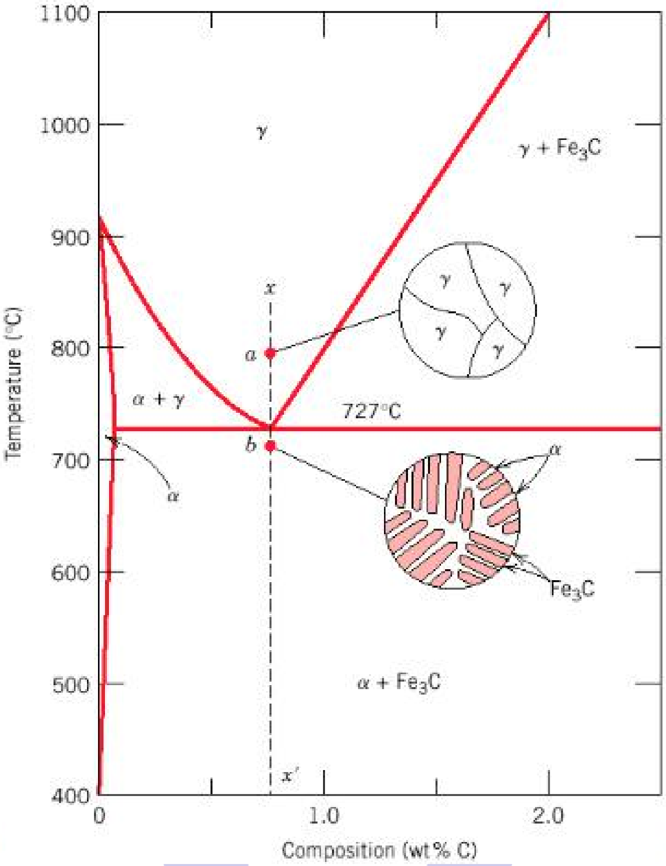


Eutectoid: 0.76 wt%C, 727 °C

$$\gamma(0.76\text{ wt\% C}) \leftrightarrow \alpha\,(0.022\text{ wt\% C}) + Fe_3C$$

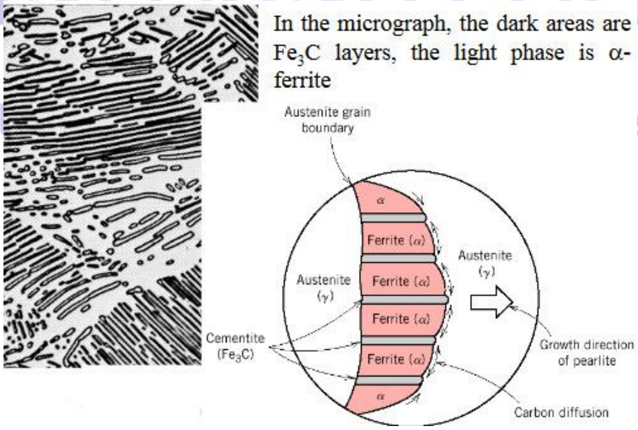
Eutectic and eutectoid reactions are very important in heat treatment of steels

Development of Microstructure in Iron - Carbon alloysMicrostructure depends on composition (carbon content) and heat treatment. In the discussion below we consider slow cooling in which equilibrium is maintained.Microstructure of eutectoid steel



Microstructure of eutectoid steel

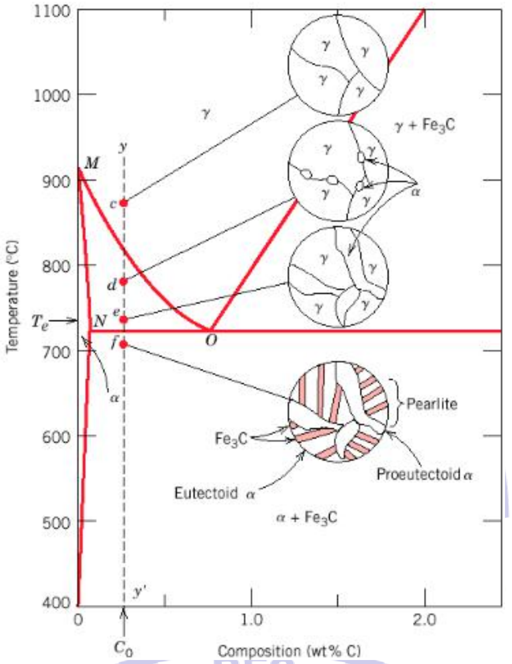
When alloy of eutectoid composition (0.76 wt % C) is cooled slowly it formspearlite, a lamellar or layered structure of two phases: α-ferrite and cementite (Fe3C)The layers of alternating phases in pearlite are formed for the same reason as layered structure of eutectic structures: redistribution C atoms between ferrite (0.022 wt%) and cementite (6.7 wt%) by atomic diffusion. Mechanically, pearlite has properties intermediate to soft, ductile ferrite and hard, brittle cementite.


In the micrograph, the dark areas are Fe_3C layers, the light phase is α-ferrite

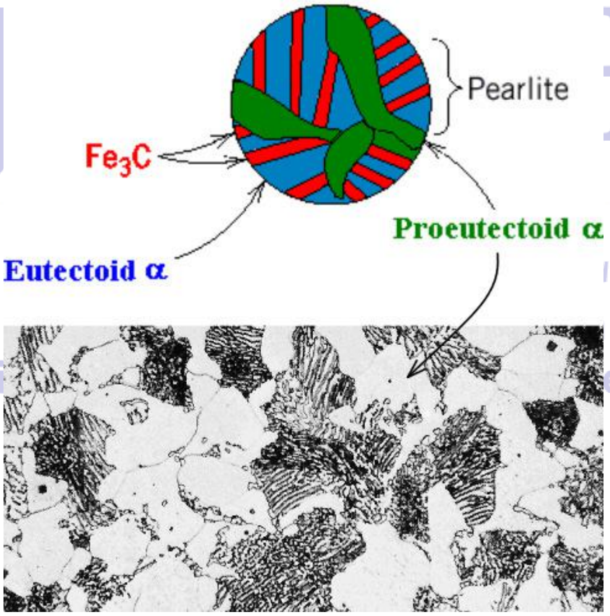
Microstructure of hypoeutectoid steel

Compositions to the left of eutectoid (0.022 - 0.76 wt % C) hypoeutectoid (less than eutectoid -Greek) alloys.

$$\gamma \rightarrow \alpha + \gamma \rightarrow \alpha + Fe_3C$$



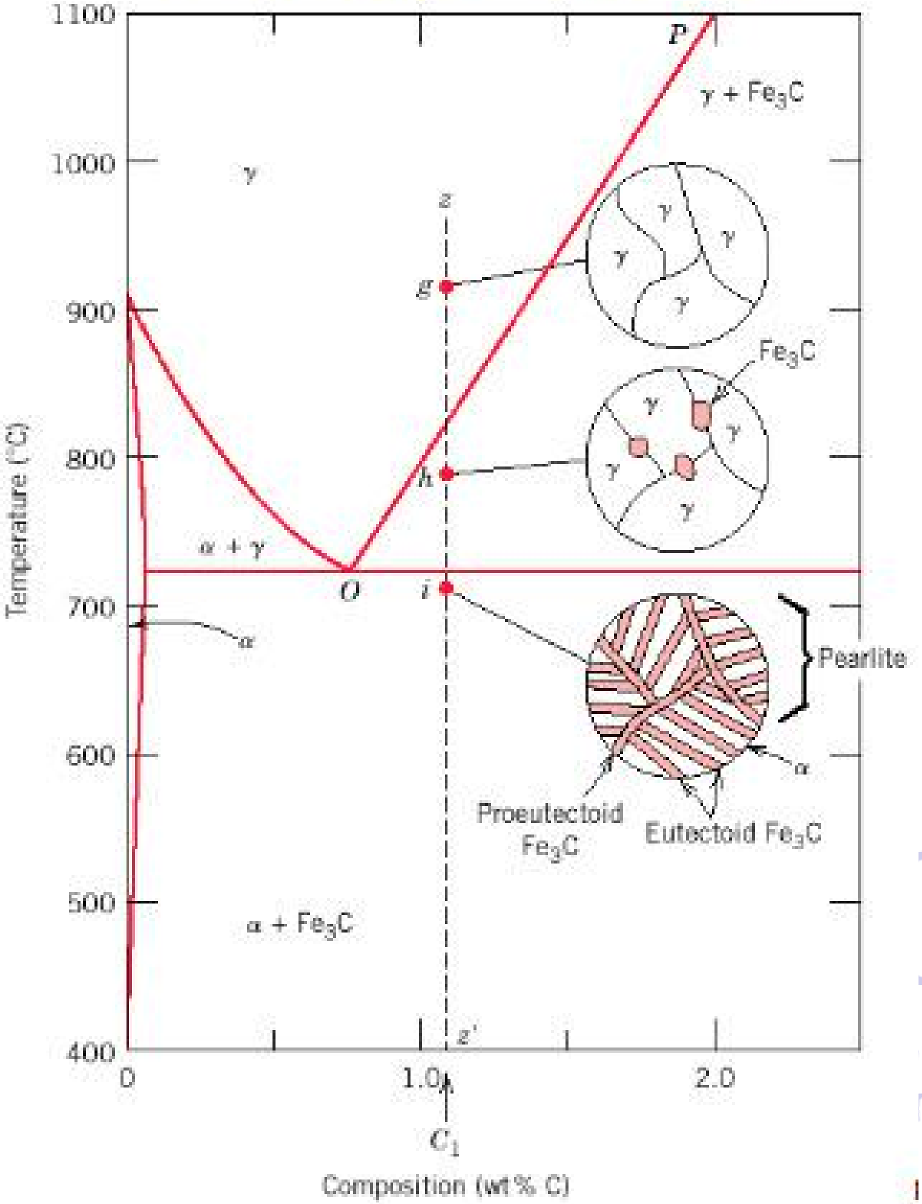
Hypoeutectoid alloys contain proeutectoid ferrite (formed above the eutectoid temperature) plus the eutectoid perlite that contain eutectoid ferrite and cementite.



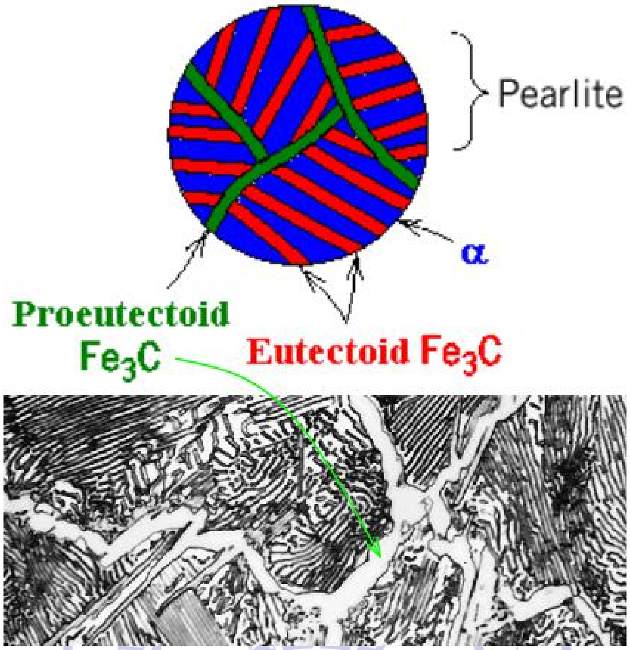
Microstructure of hypereutectoid steel

Compositions to the right of eutectoid (0.76 - 2.14 wt % C) hypereutectoid (more than eutectoid -Greek) alloys

$$\gamma \rightarrow \gamma + Fe_3C \rightarrow \alpha + Fe_3C$$

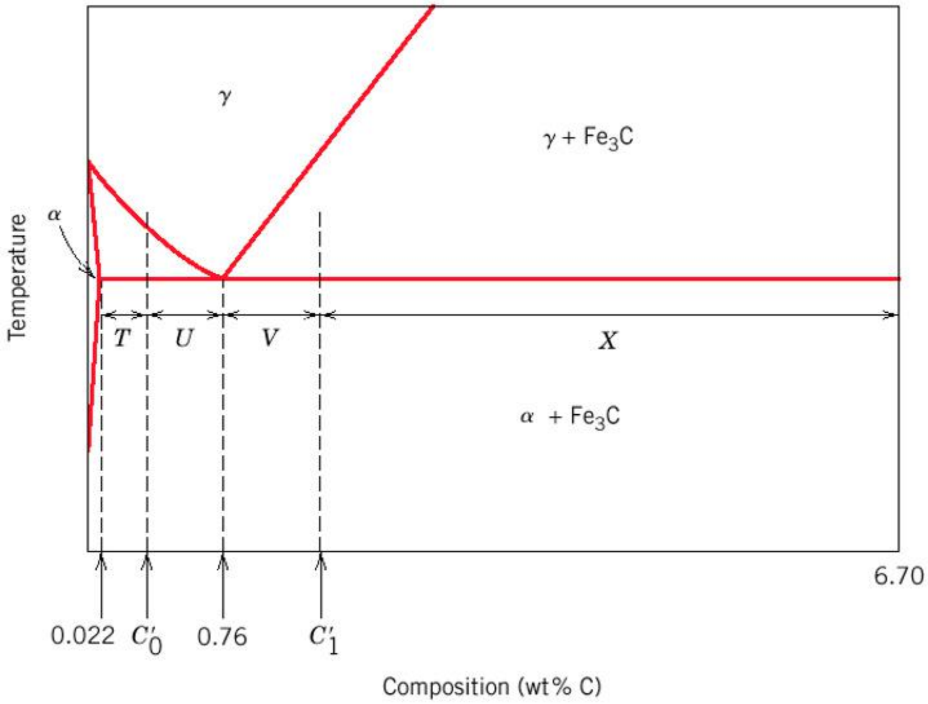


Hypereutectoid alloys contain proeutectoid cementite(formed above the eutectoid temperature) plus perlite that contain eutectoid ferrite and cementite.



How to calculate the relative amounts of proeutectoid phase (αor Fe3C) and pearlite?

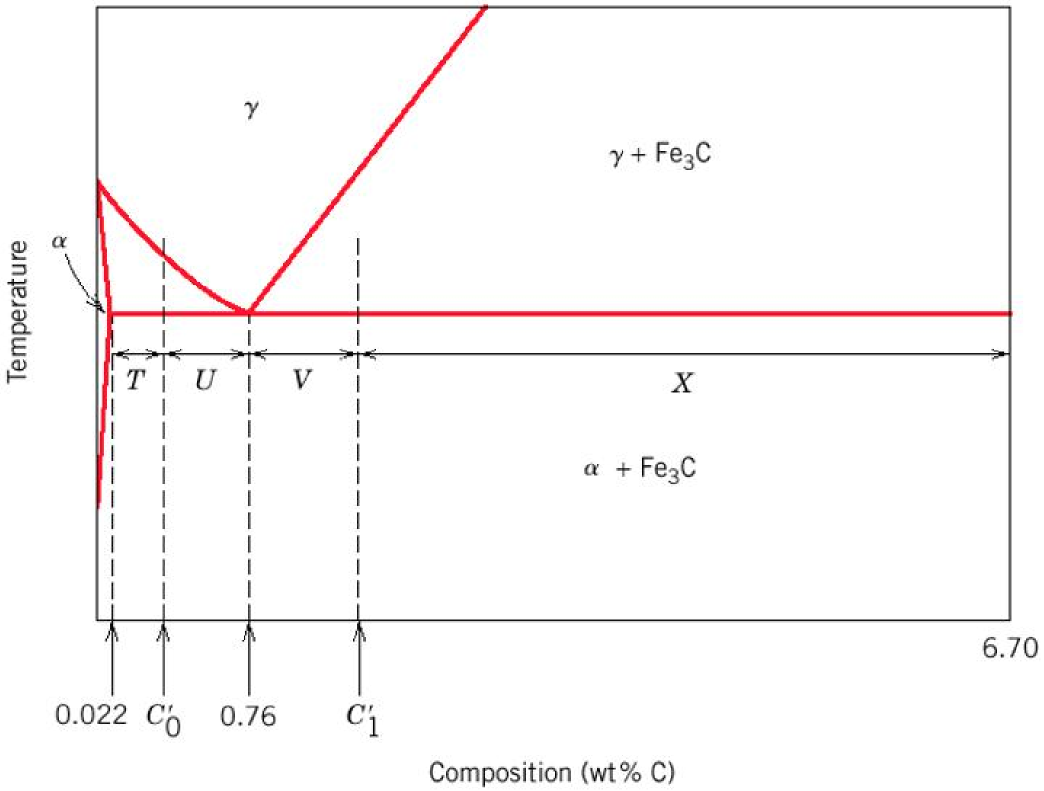
Application of the lever rule with tie line that extends from the eutectoid composition (0.76 wt% C) to α –(α + Fe3C) boundary (0.022 wt% C) for hypoeutectoid alloys and to (α + Fe3C) – Fe3C boundary (6.7 wt% C) for hypereutectoid alloys.



Fraction of α phase is determined by application of the lever rule across the entire (α+ Fe3C) phase field.

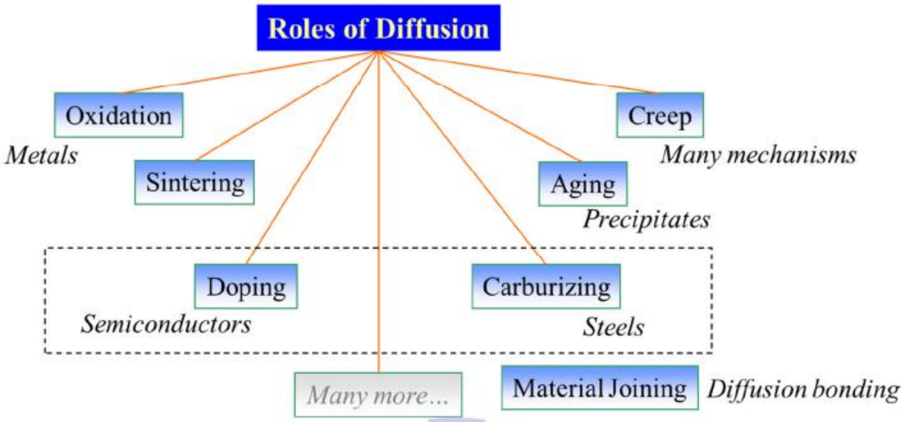
Example for hypereutectoid alloy with composition C1

Fraction of pearlite: WP = X / (V+X) = (6.7 –C1) / (6.7 –0.76) Fraction of proeutectoid cementite: WFe3C = V / (V+X) = (C1 –0.76) / (6.7 –0.76)



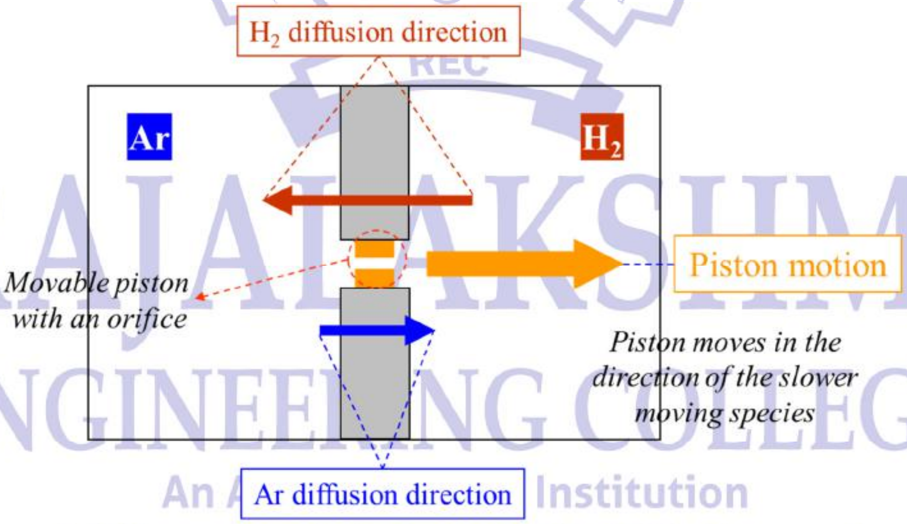
- ❑ Diffusion is relative flow of one material into another
  ➢*Mass flow process by which species change their position relative to their neighbours.*
- ❑ Diffusion of a species occurs from a region of high concentration to low concentration (usually). More accurately, diffusion occurs down the chemical potential (μ) gradient.
- ❑ To comprehend many materials related phenomenon (as in the figure below) one must understand Diffusion.
- ❑ The focus of the current chapter is solid state diffusion in crystalline materials.

In the current context, diffusion should be differentiated with flow (of usually fluids and sometime solids).



- ☐ When a perfume bottle is opened at one end of a room, its smell reaches the other end via the diffusion of the molecules of the perfume.
- ☐ If we consider an experimental setup as below (with Ar and H_2 on different sides of a chamber separated by a movable piston), H_2 will diffuse faster towards the left (as compared to Ar). As obvious, this will lead to the motion of movable piston in the direction of the slower moving species.

This experiment can be used to understand the Kirkendall effect.



- ☐ Mass flow process by which species change their position relative to their neighbours.
- ☐ Diffusion is driven by *thermal energy* and a '*gradient' (usually in chemical potential).* Gradients in other physical quantities can also lead to diffusion (as in the figure below). In this chapter we will essentially restrict ourselves to concentration gradients.
- ☐ Usually, *concentration gradients imply chemical potential gradients*; but there are exceptions to this rule. Hence, sometimes diffusion occurs 'uphill' in concentration gradients, but downhill in chemical potential gradients.
- ☐ Thermal energy leads to thermal vibrations of atoms, leading to atomic jumps.

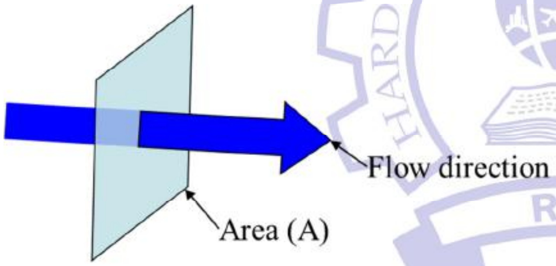
- In the absence of a gradient, atoms will still randomly ‘jump about’, without any net flow of matter.

- Concentration gradient. Concentration can be designated in many ways (e.g. moles per unit volume). Concentration gradient is the difference in concentration between two points (usually close by).

- We can use a restricted definition of flux (J) as flow per unit area per unit time:
  → mass flow / area / time → [Atoms / m^2 / s].

Steady state. The properties at a single point in the system does not change with time. These properties in the case of fluid flow are pressure, temperature, velocity and mass flow rate.
▪ In the context of diffusion, steady state usually implies that, concentration of a given species at a given point in space, does not change with time.

- In diffusion problems, we would typically like to address one of the following problems.
  (i) What is the composition profile after a contain time (i.e. determine c(x,t))?



$$J = \frac{1}{A}\frac{dn}{dt}$$

$$J \rightarrow \left[\frac{mass}{area \cdot time}\right] = \left[\frac{atoms}{m^2 \cdot s}\right]$$

Fick’s I law

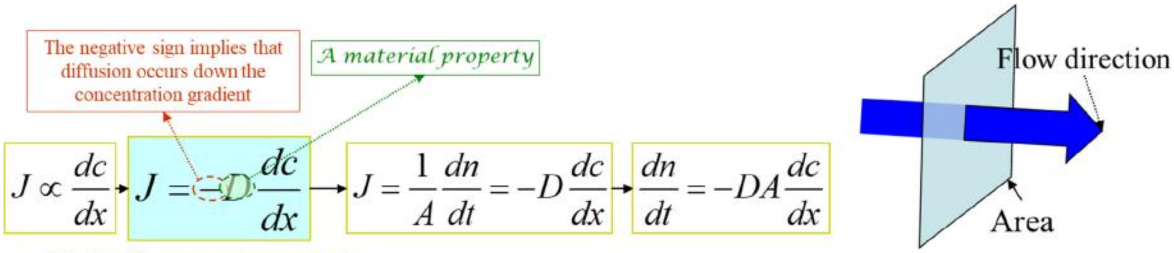
- Assume that only species ‘S’ is moving across an area ‘A’. Concentration gradient for species ‘S’ exists across the plane.

- The concentration gradient *(dc/dx)* drives the flux *(J)* of atoms.

- Flux (J) is assumed to be proportional to concentration gradient.

- The constant of proportionality is the Diffusivity or Diffusion Coefficient (D).
  ▪ ‘D’ is assumed to be independent of the concentration gradient.
  ▪ Diffusivity is a material property. It is a function of the composition of the material and the temperature.
  ▪ In crystals with cubic symmetry the diffusivity is isotropic (i.e. does not depend on direction).

- Even if steady state conditions do not exist (concentration at a point is changing with time, there is accumulation/depletion of matter), Fick’s I-equation is *still valid* (but not easy to use).

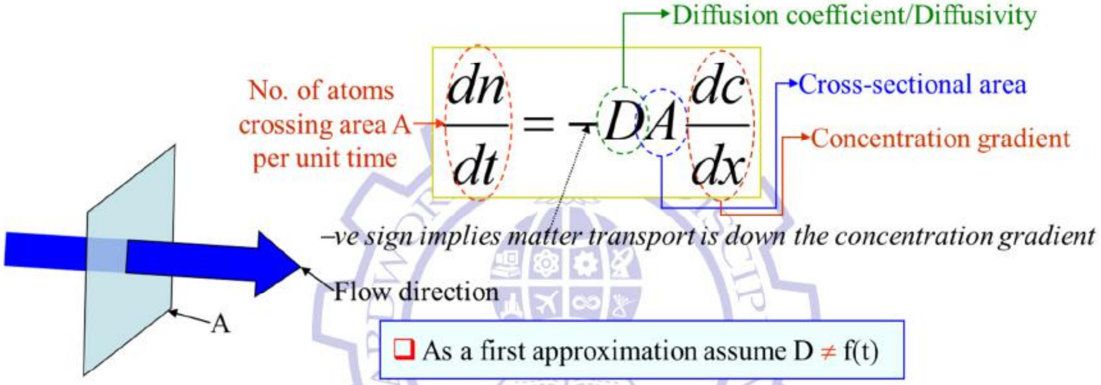


The negative sign implies that diffusion occurs down the concentration gradient

A material property

$$J \propto \frac{dc}{dx} \rightarrow J = -D\frac{dc}{dx} \rightarrow J = \frac{1}{A}\frac{dn}{dt} = -D\frac{dc}{dx} \rightarrow \frac{dn}{dt} = -DA\frac{dc}{dx}$$

Fick's first law (equation)



Diffusion coefficient/Diffusivity

No. of atoms crossing area A per unit time

$$\frac{dn}{dt} = -DA\frac{dc}{dx}$$

Cross-sectional area

Concentration gradient

–ve sign implies matter transport is down the concentration gradient

❑ As a first approximation assume $D \neq f(t)$

Let us look at the units of Diffusivity

$$\left\{J = -D\frac{dc}{dx}\right\} \rightarrow \left[\frac{number}{m^2\,s}\right] = [D]\left[\frac{number}{m^3}\cdot\frac{1}{m}\right]$$

$$\left[\frac{m^2}{s}\right] = [D]$$

Note the strange unit of D: [m^2/s]

Fick's II law

- ❑ The equation as below is often refered to as the Fick's II law (though clearly this is an equation and not a law).
- ❑ This equation is derived using Fick's I-equation and mass balance.
- ❑ The equation is a second order PDE requiring one initial condition and two boundary conditions to solve.

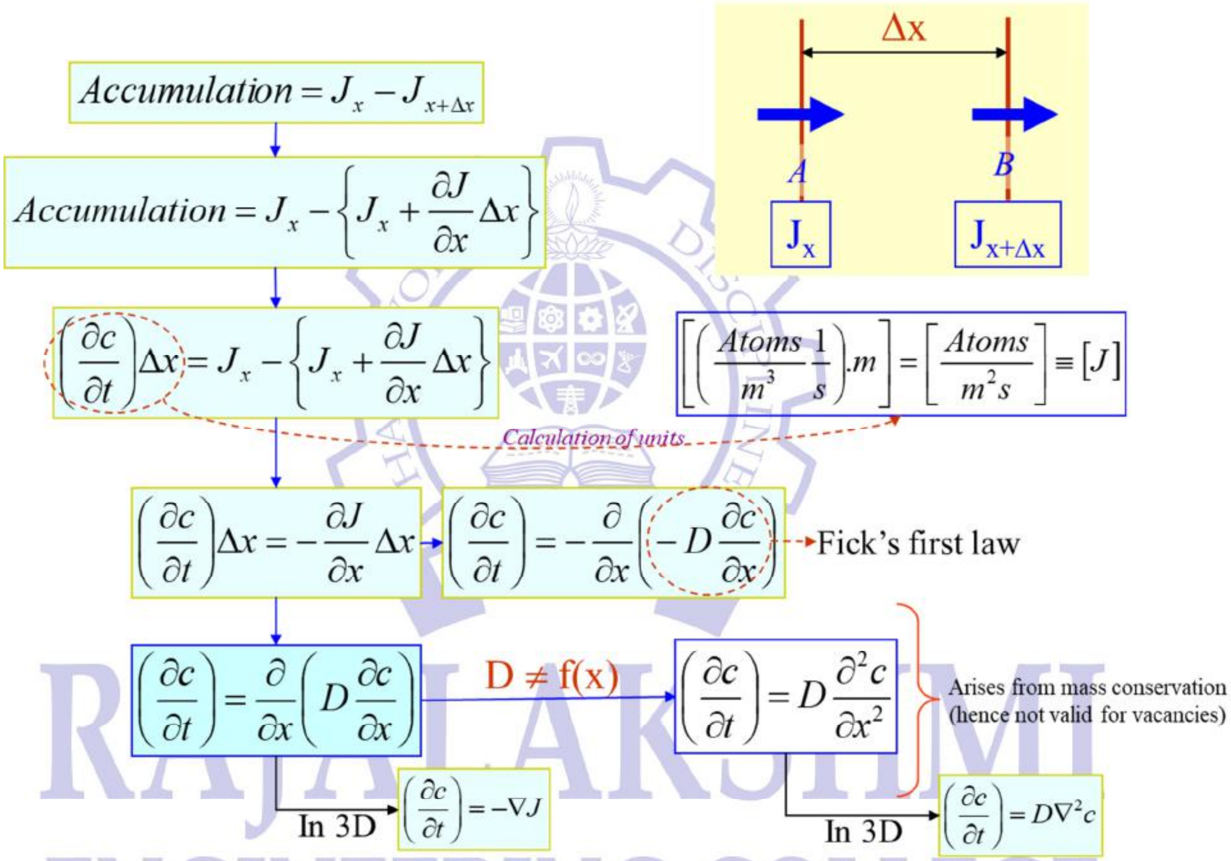
$$\left(\frac{\partial c}{\partial t}\right) = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)$$

Derivation of this equation will taken up next.

- ❑ If 'D' is not a function of the position, then it can be 'pulled out'.

$$\boxed{\left(\frac{\partial c}{\partial t}\right) = D\frac{\partial^2 c}{\partial x^2}}$$

- ☐ If J_x is the flux arriving at plane A and $J_{x+\Delta x}$ is the flux leaving plane B. Then the Accumulation of matter is given by: $(J_x - J_{x+\Delta x})$.



$$Accumulation = J_x - J_{x+\Delta x}$$

$$Accumulation = J_x - \left\{J_x + \frac{\partial J}{\partial x}\Delta x\right\}$$

$$\left(\frac{\partial c}{\partial t}\right)\Delta x = J_x - \left\{J_x + \frac{\partial J}{\partial x}\Delta x\right\}$$

Calculation of units

$$\left[\left(\frac{Atoms}{m^3}\frac{1}{s}\right).m\right] = \left[\frac{Atoms}{m^2 s}\right] \equiv [J]$$

$$\left(\frac{\partial c}{\partial t}\right)\Delta x = -\frac{\partial J}{\partial x}\Delta x \rightarrow \left(\frac{\partial c}{\partial t}\right) = -\frac{\partial}{\partial x}\left(-D\frac{\partial c}{\partial x}\right)$$

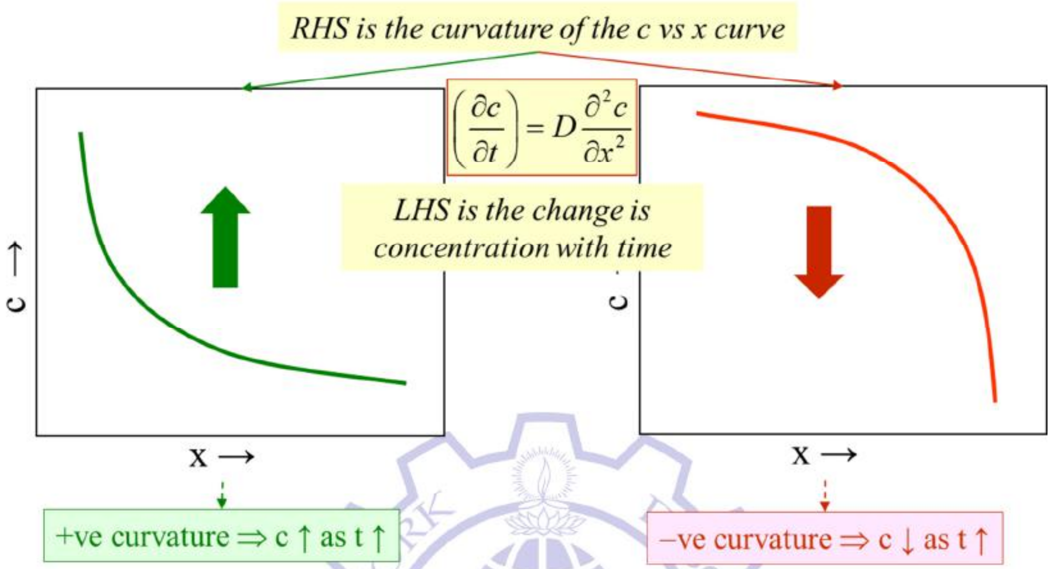
Fick's first law

$$\left(\frac{\partial c}{\partial t}\right) = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) \xrightarrow{D \neq f(x)} \left(\frac{\partial c}{\partial t}\right) = D\frac{\partial^2 c}{\partial x^2}$$

Arises from mass conservation (hence not valid for vacancies)

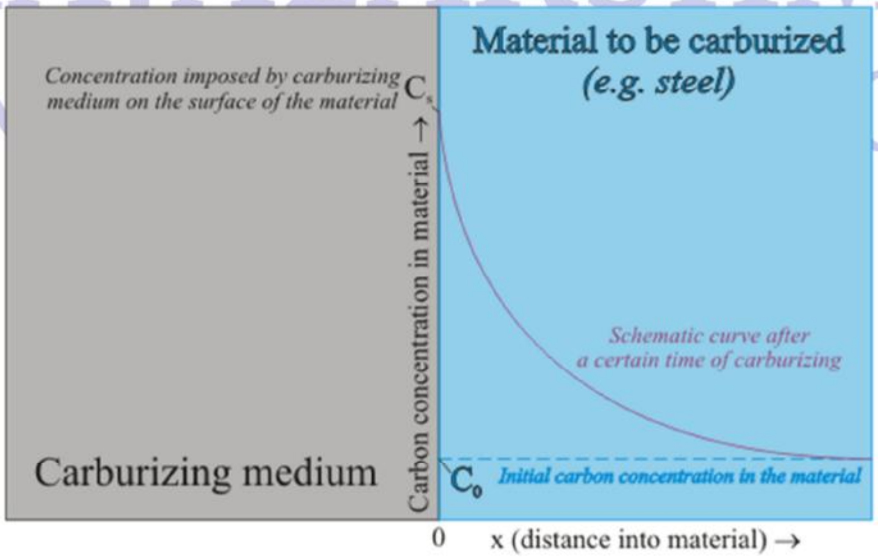
In 3D $$\left(\frac{\partial c}{\partial t}\right) = -\nabla J$$

In 3D $$\left(\frac{\partial c}{\partial t}\right) = D\nabla^2 c$$



Applications based on Fick's II law (*Carburization of steel)*

- Surface is often the most important part of the component, which is prone to degradation.
- Surface hardening of steel components like gears is done by carburizing or nitriding.
- Carburizing is done in the γ-phase field, where in the solubility of carbon is higher that that in the α phase. The high temperature enhances the kinetics as well.
- In pack carburizing, a solid carbon powder used as C source.
- In gas carburizing Methane gas is used a carbon source using the following reaction. CH_4 (g) → $2H_2$ (g) + C (the carbon released diffuses into steel).



It is usually assumed that the carbon concentration on the surface (C_S) is constant (i.e. the carburizing medium imposes a constant concentration on the surface). An uniform homogeneous carbon concentration (C_0) is assumed in the material before the carburization. Transient diffusion conditions exist and C diffuses into the steel.

Theory of Homogeneous Nucleation

At the very first stage of phase transition at a particular super-saturation a few no. of small-sized nuclei (cluster) of new phase is generated in the sea of old meta-stable phase. To undergo phase transition the system needs to cross a barrier at a certain cluster size which is called critical cluster size. This barrier crossing is activated process and is accompanied by thermal fluctuation of cluster size. Once system crosses this barrier the size of the critical cluster starts growing spontaneously and leads to the phase transition. The first activated process is called "nucleation" whereas the second spontaneous step is known as "growth". Although nucleation is initiated by local fluctuation of order parameter (such as density in case of gas-liquid condensation), to cross the barrier it needs a large thermal fluctuation which is rare at small super-saturation or super cooling. However, as super-cooling/super-saturation is increased, the height of barrier decreases, and at some well-defined value of the super cooling/super saturation the barrier height becomes comparable to the magnitude of the thermal fluctuation, and the formation of the new phase becomes rapid.

Let us consider a liquid drop formed in a super cooled vapor of the same substance starting from homogeneous vapor phase. We consider the situation where the drop is in equilibrium with the vapor. Now, we want to calculate the free energy difference due to formation of the liquid drop.

Let, ΔG_v be the bulk free energy difference to obtain a liquid drop of unit volume.

Then the free energy to formation a liquid drop of radius 'r' is given by,

$$\Delta G = -\frac{4\pi}{3} r^3 \Delta G_v + 4\pi r^2 \gamma$$

where 'γ' is the surface tension of liquid-gas interface

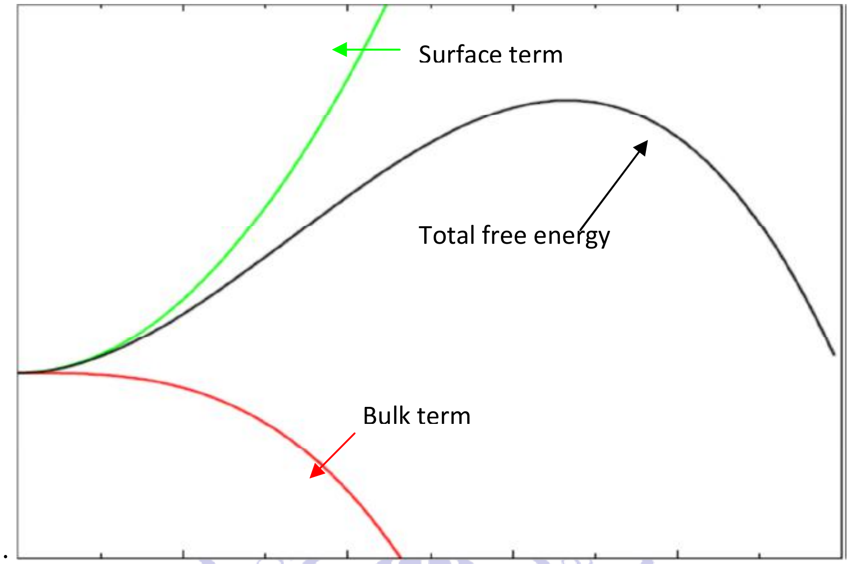


figure1: free energy of nucleation as a function of radius of nucleus (green line is surface free energy, red is bulk and black line is total free energy of formation)

This function is sketched in fig. It has a maximum at r^*, where

$$r^* = \frac{2\gamma}{\Delta G_v}$$

and the value of ΔG corresponding to this maximum is,

$$\Delta G^* = \frac{16\pi}{3}\frac{\gamma^3}{(\Delta G_v)^2}$$

Note that as super cooling ΔT increases, ΔG^* decreases, as ΔG increases and γ does not change with increasing super cooling.

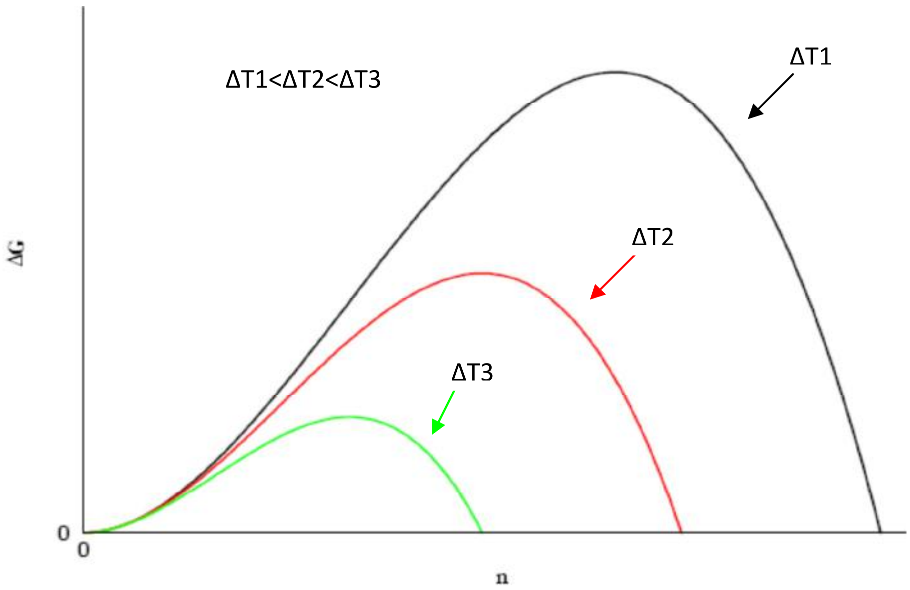


figure2: free energy at different super-cooling (ΔT)

Since the nucleation is an thermally activated process this is the slowest and rate determining step of phase transition. In other words, the formation of a droplet of critical size constitutes the bottleneck of the whole phase transition process.

Assuming that an equilibrium embryo distribution is maintained at any stage of super cooling one can correlate the population of nuclei of critical size. The no. of embryo of size 'k' is given by,

$$n_k = n_0 \exp(-\frac{\Delta G}{k_B T})$$

where 'n_0' is the total no. of particles.

Phase Transformations of Fe-C (a review)

Phase Transformation: Kinetics

Phase transformations (change of the microstructure) can be divided into three categories: Phase transformations. Kinetics.

- Diffusion-dependent with no change in phase composition or number of phases present (e.g. melting, solidification of pure metal, allotropic transformations, recrystallization, etc.)
- Diffusion-dependent with changes in phase compositions and/or number of phases (e.g. eutectoid transformations)

- Diffusion less phase transformation - produces a metastable phase by cooperative small displacements of all atoms in structure (e.g. martensitic transformation discussed in later in this chapter)

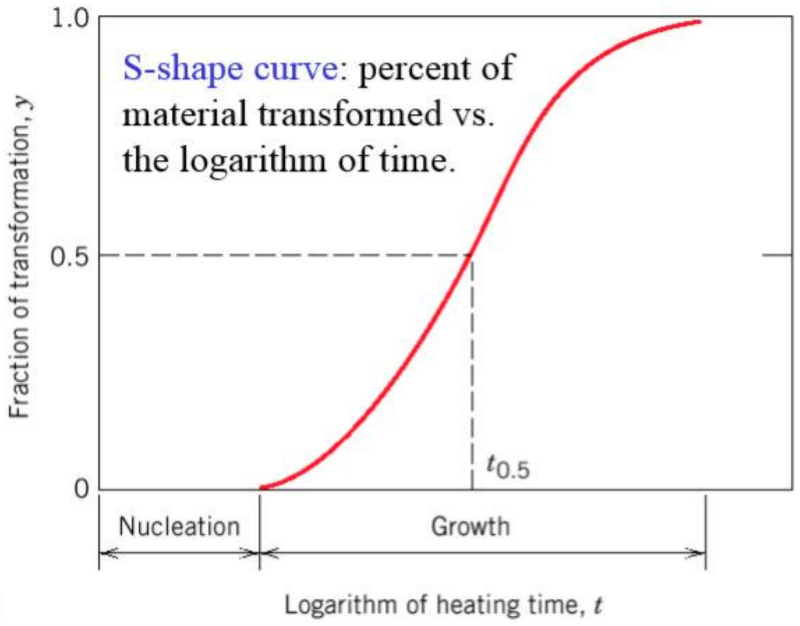
Phase transformations do not occur instantaneously. Diffusion-dependent phase transformations can be rather slow and the final structure often depend on the rate of cooling/heating. We need to consider the time dependence or kinetics of the phase transformations.

Most phase transformations involve change in composition ⇒redistribution of atoms via diffusion is required. The process of phase transformation involves:

Kinetics of phase transformations

- Nucleation of the new phase - formation of stable small particles (nuclei) of the new phase. Nuclei are often formed at grain boundaries and other defects.
- Growth of new phase at the expense of the original phase.

$$y = 1 - \exp(-kt^n)$$ **Avrami Equation**

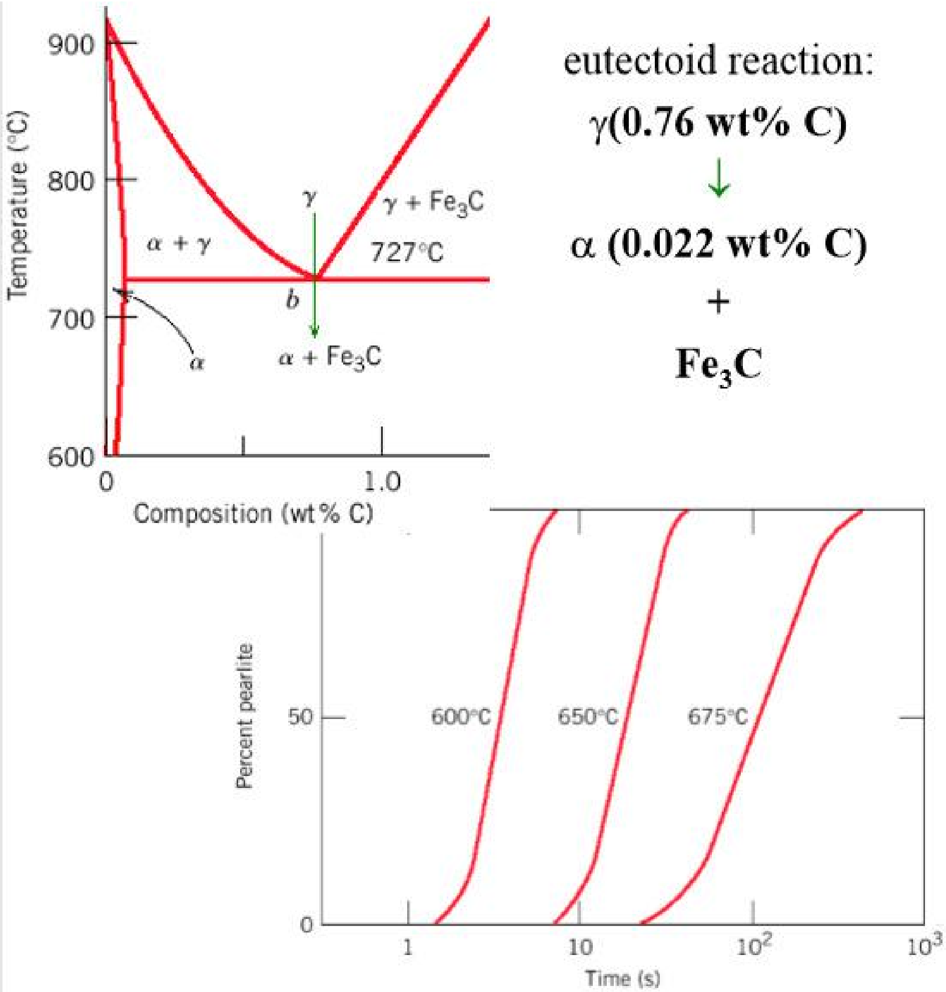


Superheating / supercooling

- Upon crossing a phase boundary on the compositiontemperature phase diagram phase transformation towards equilibrium state is induced.
- But the transition to the equilibrium structure takes time and transformation is delayed.
- During cooling, transformations occur at temperatures less than predicted by phase diagram: supercooling.
- During heating, transformations occur at temperatures greater than predicted by phase diagram: superheating.
- Degree of supercooling/superheating increases with rate of cooling/heating.
- Metastable states can be formed as a result of fast temperature change. Microstructure is strongly affected by the rate of cooling.

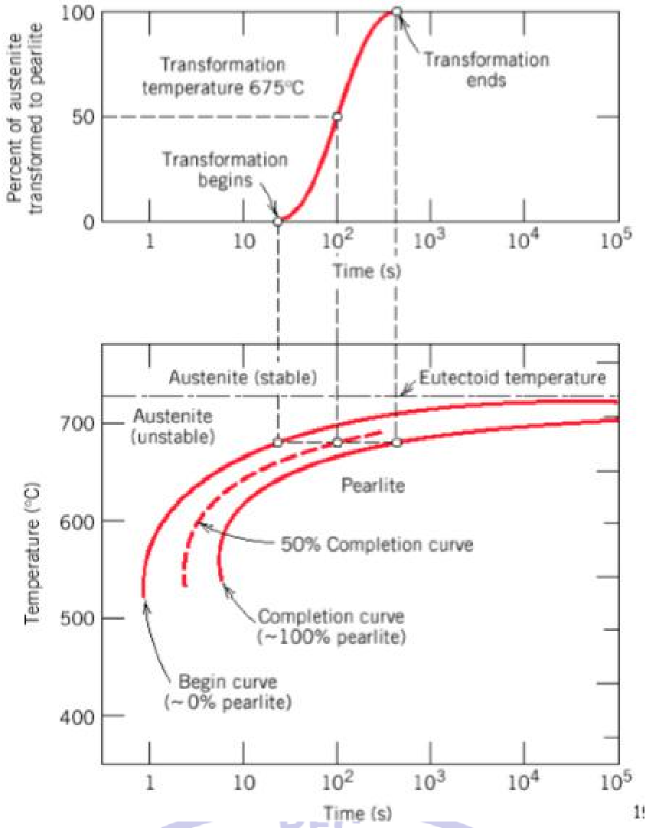
- Below we will consider the effect of time on phase transformations using iron-carbon alloy as an example.

Let us consider eutectoid reaction as an example

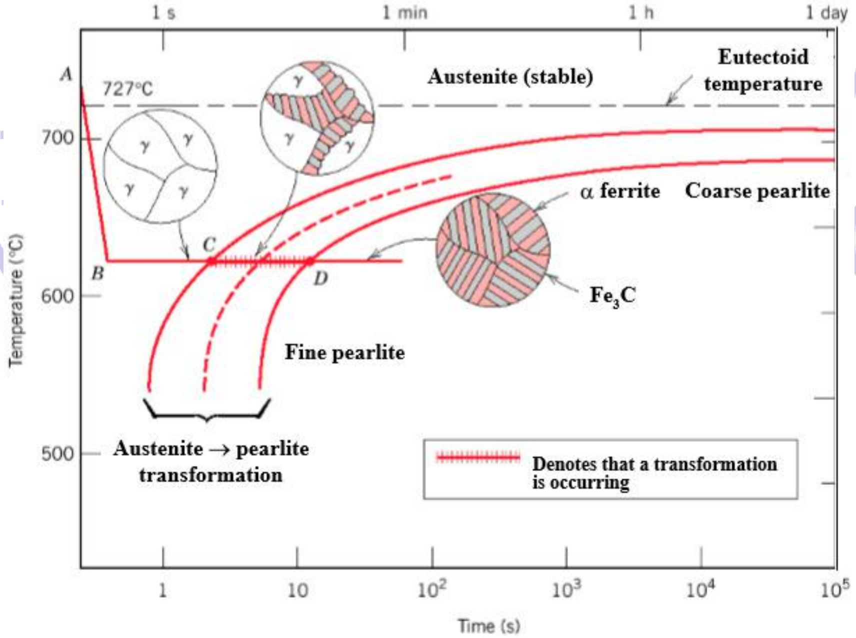


The S-shaped curves are shifted to longer times at higher T showing that the transformation is dominated by nucleation (nucleation rate increases with supercooling) and not by diffusion (which occurs faster at higher T).

Isothermal Transformation (or TTT) Diagrams (Temperature, Time, and % Transformation)



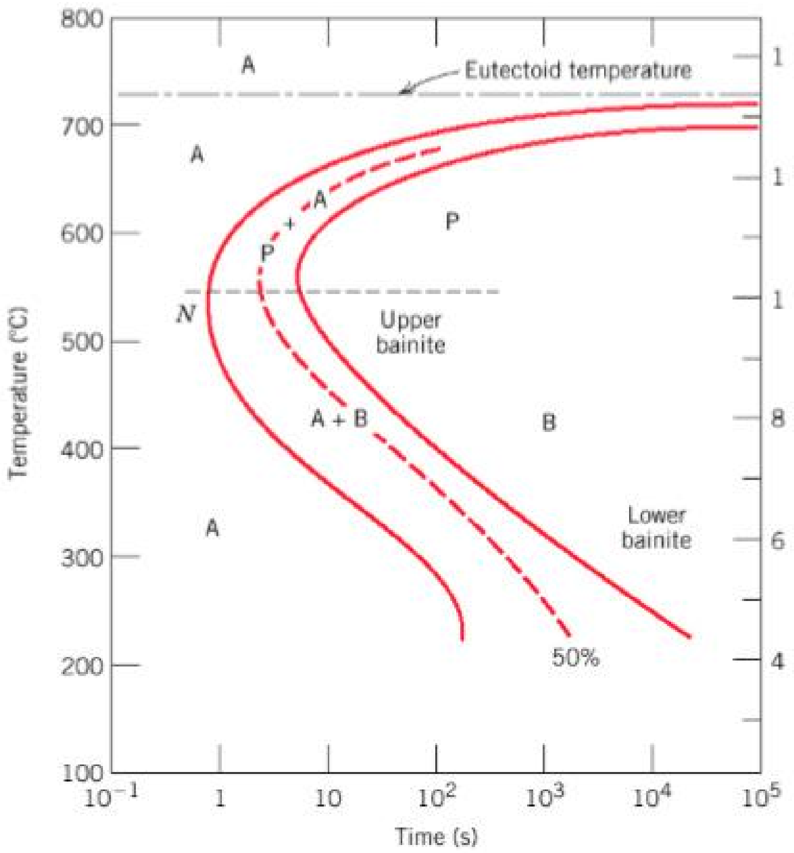
TTT Diagrams



The thickness of the ferrite and cementite layers in pearlite is ~ 8:1. The absolute layer thickness depends on the temperature of the transformation. The higher the temperature, the thicker the layers.

- The family of S-shaped curves at different T are used to construct the TTT diagrams.
- The TTT diagrams are for the isothermal (constant T) transformations (material is cooled quickly to a given temperature before the transformation occurs, and then keep it at that temperature).
- At low temperatures, the transformation occurs sooner (it is controlled by the rate of nucleation) and grain growth (that is controlled by diffusion) is reduced.
- Slow diffusion at low temperatures leads to fine-grained microstructure with thin-layered structure of pearlite (fine pearlite).
- At higher temperatures, high diffusion rates allow for larger grain growth and formation of thick layered structure of pearlite (coarse pearlite).
- At compositions other than eutectoid, a proeutectoid phase (ferrite or cementite) coexist with pearlite. Additional curves for proeutectoid transformation must be included on TTT diagrams.

Formation of Bainite Microstructure (I)

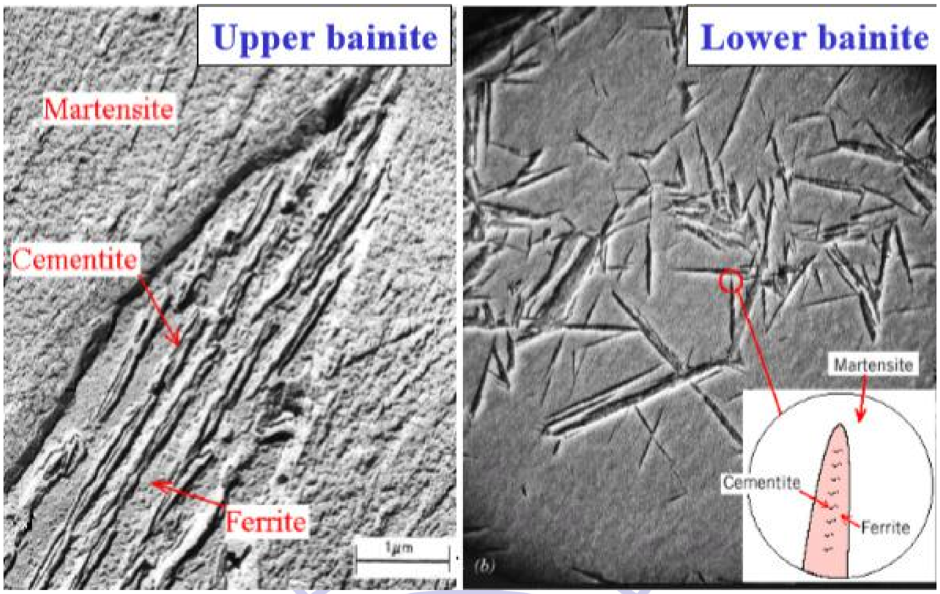


If transformation temperature is low enough (≤540°C) bainite rather than fine pearlite forms.

Formation of Bainite Microstructure

- For T ~ 300-540°C, upper bainite consists of needles of ferrite separated by long cementite particles
- For T ~ 200-300°C, lower bainite consists of thin plates of ferrite containing very fine rods or blades of cementite

- In the bainite region, transformation rate is controlled by microstructure growth (diffusion) rather than nucleation. Since diffusion is slow at low temperatures, this phase has a very fine (microscopic) microstructure.
- Pearlite and bainite transformations are competitive; transformation between pearlite and bainite not possible without first reheating to form austenite.



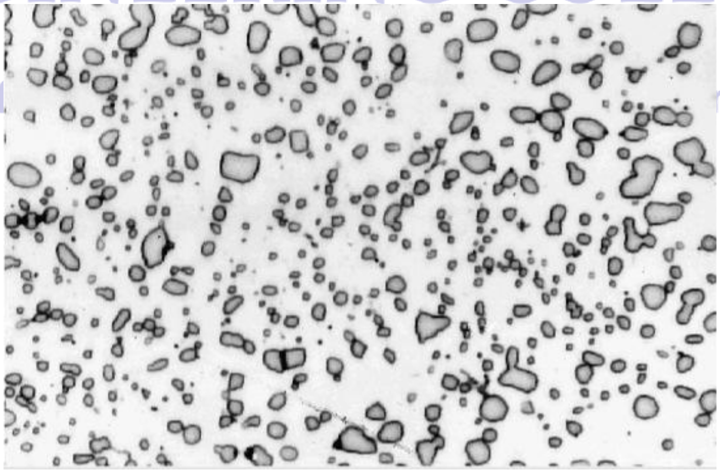
Spheroidite

• Annealing of pearlitic or bainitic microstructures at elevated temperatures just below eutectoid (e.g. 24 h at 700 C) leads to the formation of new microstructure – spheroidite-spheres of cementite in a ferrite matrix.

• Composition or relative amounts of ferrite and cementite are not changing in this transformation, only shape of the cementite inclusions is changing.

• Transformation proceeds by C diffusion –needs high T.

• Driving force for the transformation - reduction in total ferrite -cementite boundary area



Martensite

- Martensite forms when austenite is rapidly cooled (quenched) to room Temperature.

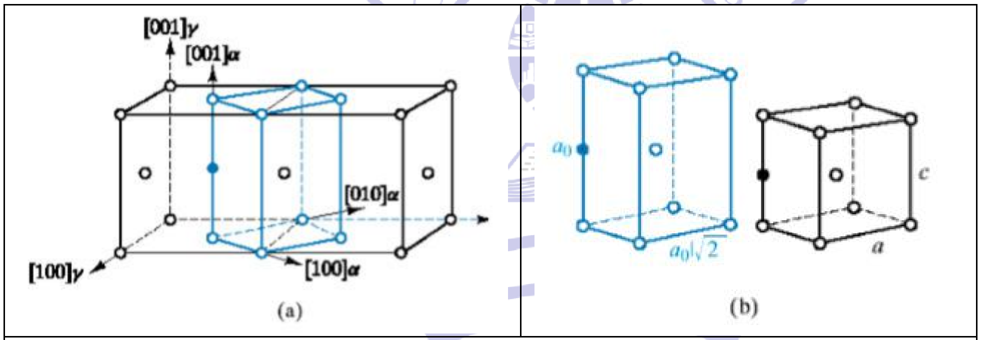
- It forms nearly instantaneously when the required low temperature is reached. The austenite-martensite does not involve diffusion → no thermal activation is needed, this is called an athermal transformation.

- Each atom displaces a small (sub-atomic) distance to transform FCC γ-Fe (austenite)to martensite which has a Body Centered Tetragonal (BCT) unit cell (like BCC, but one unit cell axis is longer than the other two).

- Martensite is metastable - can persist indefinitely at room temperature, but will transform to equilibrium phases on annealing at an elevated temperature.

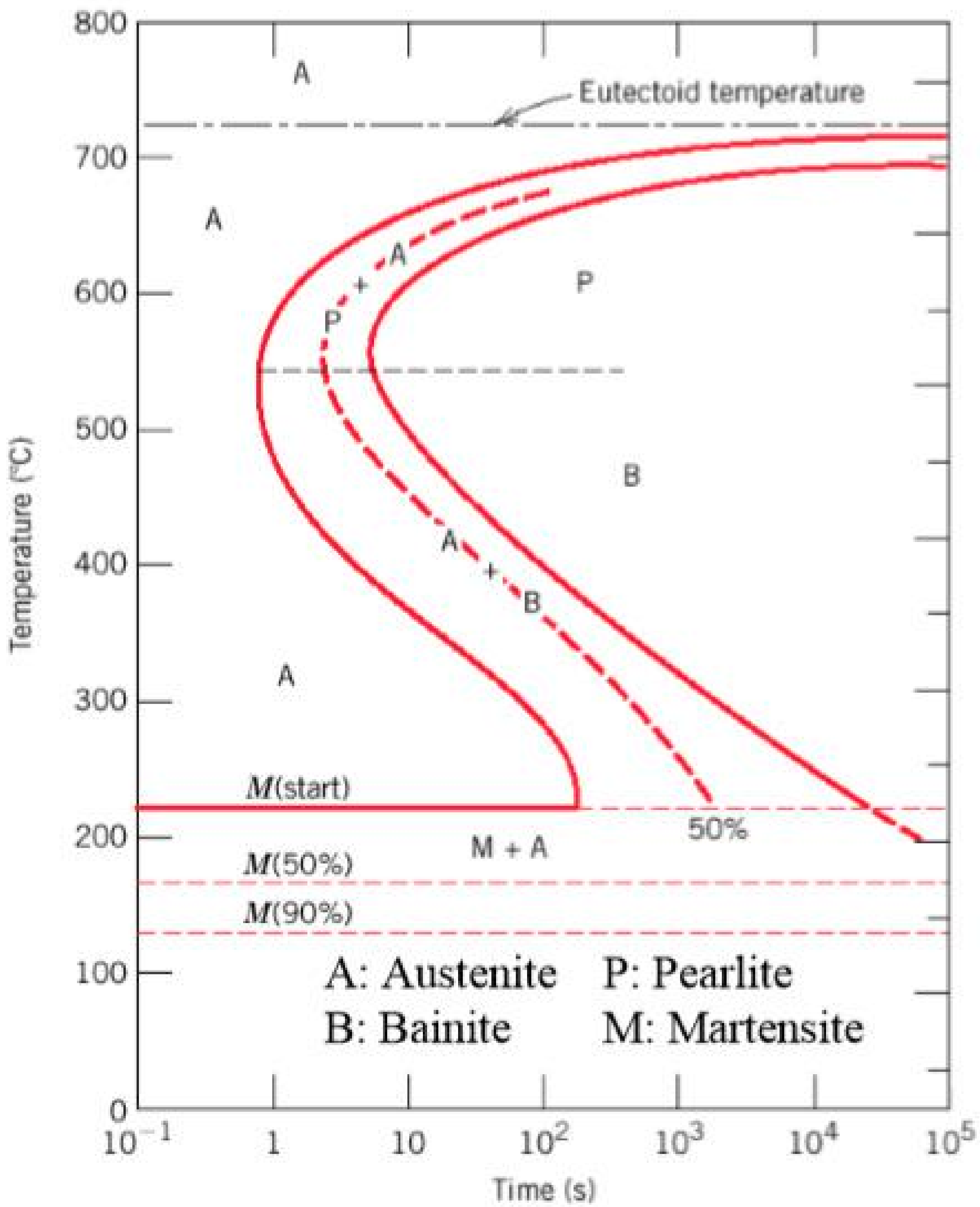
- Martensite can coexist with other phases and/or microstructures in Fe-C system

- Since martensite is metastable non-equilibrium phase, it does not appear in phase Fe-C phase diagram



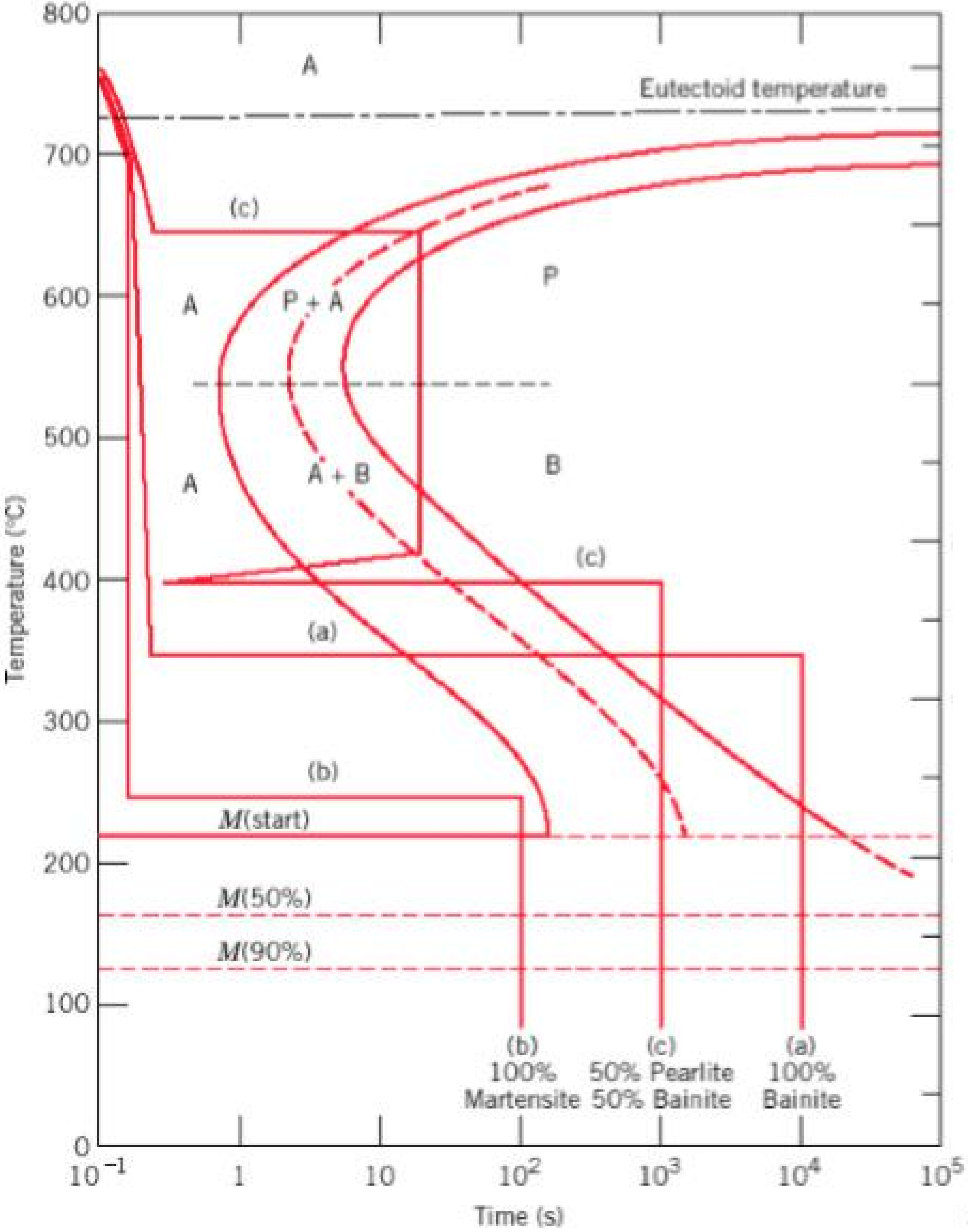
The martensitic transformation involves the sudden reorientation of C and Fe atoms from the FCC solid solution of γ-Fe (austenite) to a body-centered tetragonal (BCT) solid solution (martensite).

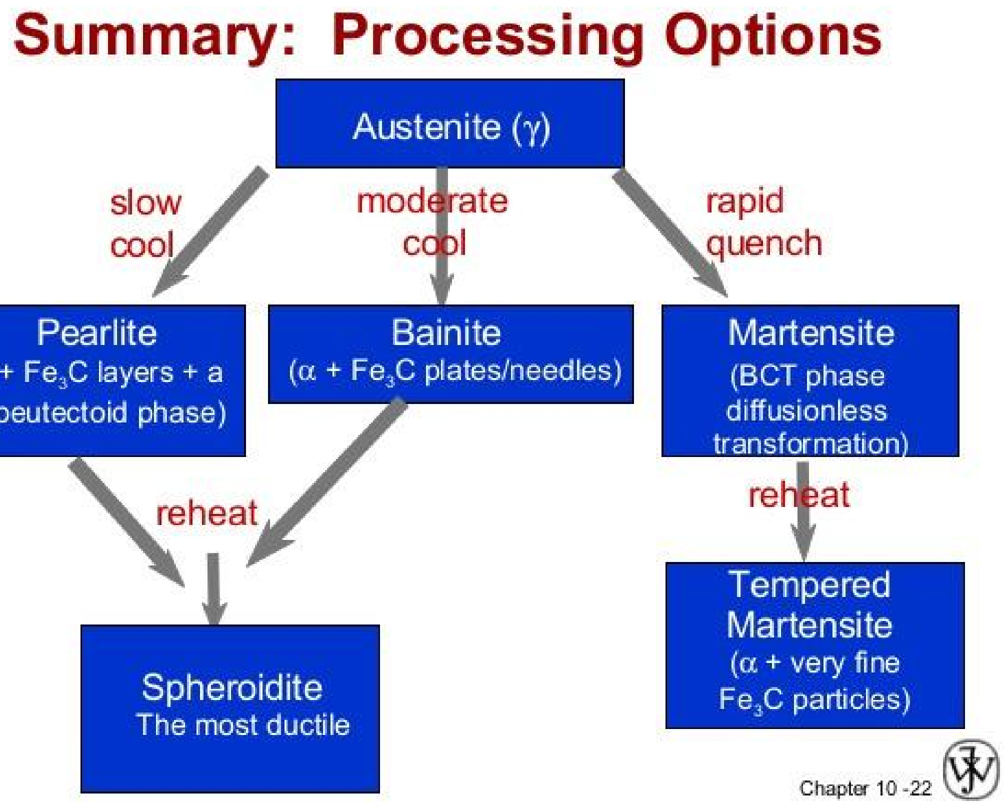
TTT Diagram including Martensite



Austenite-to-martensite is diffusion less and very fast. The amount of martensite formed depends on temperature only.

Time-temperature path –microstructure


A
Eutectoid temperature
(c)
A
P + A
P
A
A + B
B
(c)
(a)
(b)
M(start)
M(50%)
M(90%)
(b)
100%
Martensite
(c)
50% Pearlite
50% Bainite
(a)
100%
Bainite
Temperature (°C)
800
700
600
500
400
300
200
100
0
10^{-1}
1
10
10^2
10^3
10^4
10^5
Time (s)



Summary: Processing Options

Austenite (γ)

slow cool → **Pearlite** (α + Fe_3C layers + a proeutectoid phase)

moderate cool → **Bainite** (α + Fe_3C plates/needles)

rapid quench → **Martensite** (BCT phase diffusionless transformation)

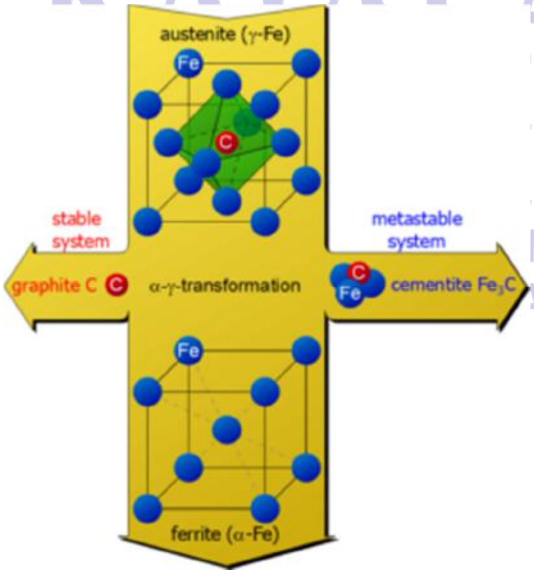
Pearlite, Bainite — reheat → **Spheroidite** The most ductile

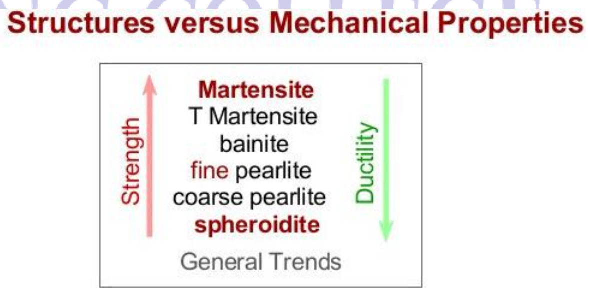
Martensite — reheat → **Tempered Martensite** (α + very fine Fe_3C particles)

Chapter 10 -22

Summary of austenite transformations

Solid lines are diffusional transformations, dashed is diffusion less martensitic transformation





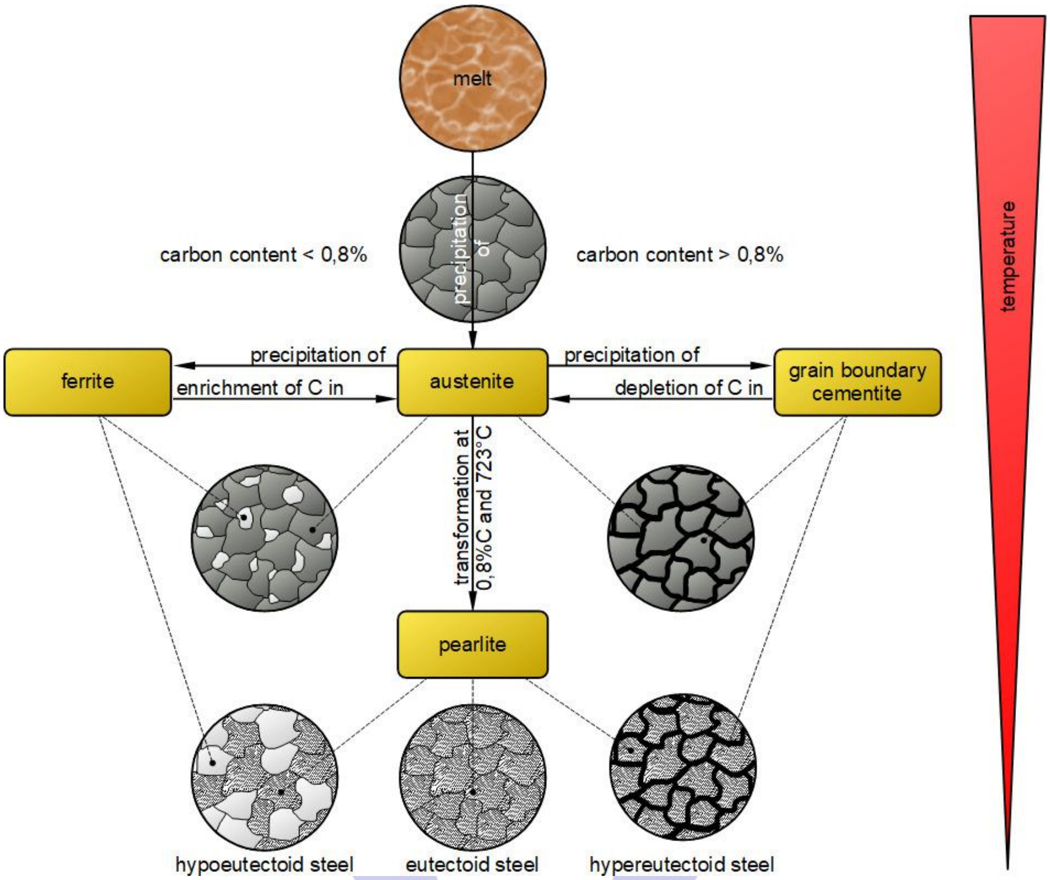
Structures versus Mechanical Properties

Strength

Martensite
T Martensite
bainite
fine pearlite
coarse pearlite
spheroidite

Ductility

General Trends



Overview of the microstructure formation of steels

The actual solidification process in steels takes place independently of the carbon content as in a solid solution alloy (typically lenticular two-phase region between the liquidus and solidus line). During solidification or immediately thereafter, the carbon is completely soluble in the face-centered cubic γ-iron lattice structure. This solid solution of iron and embedded carbon in the middle of the cube of the elementary cell is called *austenite*.

UNIT-IV

Engineering Materials and Testing

Introduction:

Material Science is a branch of science which deals with the properties of materials.

The continuous developments in the field of science and engineering open the way to new technologies and applications. Scientists and technologists are finding out new materials for high-tech applications.

The fast growing fields such as electronics, photonics, photoelasticity, fiber optics and laser technology require efficient and stable new materials.

Hence, they must posses novel properties like large optical non-linearities, opto electronic property, high sensitivity to light and large thermal and electrical conductivites. They should also have good mechanical strength, toughness, ductility, and lightness.

Materials used in high tech applications are usually designed for maximum performance and they are normally expensive. Examples of such materials include titanium alloys for supersonic airplanes, magnetic alloys for computer discs, special ceramics for the heat shield of space shuttle etc.

Let us discuss some of the newly developed engineering materials, their properties and applications.

Metallic Glasses

Mettallic glasses are **high strength**, **good magnetic properties** and **better corrosion resistance**.

Metals are solids, which exhibits ***crystalline*** property,***malleability (flexible)***, ***ductility (ability to deform under stress)*** etc.

Glasses are solids in the ***amorphous*** form in which the atoms arrangement are not periodic and they are irregular.They are ***transparent***, ***brittle (breakable)***, ***non-magnetic*** in nature.

So the Metallic glasses share the properties of **both metals and glasses**.

Metallic glasses are ***strong***, ***ductile***, ***malleable***, ***opaque*** and ***amorphous***.They have **good magnetic properties** and **high corrosion resistance**.

Metallic glass = Amorphous metal

Glass transition Temperature (Tg)

Temperature at which the **liquid** like atomic configuration canbe **frozen into a solid** is known as ***glass transition temperature.***
Glass transition temperature for metallic alloys is about **20°C to 300°C.**

Types of Metallic Glasses

Metallic glasses are of two types. They are
i. **Metal - Metalloid glasses** :
(Fe, Co, Ni) - (B, Si, C, P)
ii. **Metal - Metal glasses** :
(Ni - Nb, Mg - Zn, Cu - Zr, Hf - Va alloys)

Production of Metallic Glasses

i. Twin roller system
Molten alloy is ***passed through*** two rollers rotating in***opposite directions***.

ii. Melt spinning system - Quenching
Molten alloy jet ***impinges*** on a ***fast rotating roller***.

iii. Melt extraction system
Fast moving roller sweeps off molten droplet into a strip from a solid rod.

Melt Spinning Method

Principle

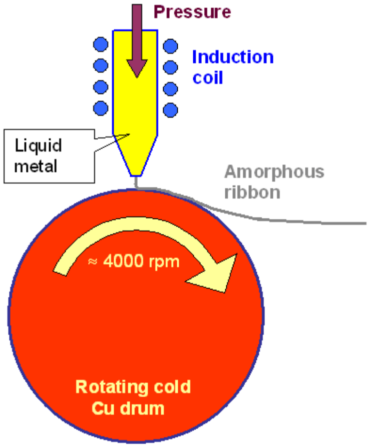
"**Quenching**" is a technique used to form metallic glasses.
Quenching means **rapid cooling**.

Actually **atoms** of any materials **move freely** in a **liquid state**.
Atoms can be **arranged regularly** when a **liquid is cooled slowly**.

Instead, when a **liquid is quenched**, there will be an **irregularpattern**, which results in the formation of **metallic glasses.**

Experimental Setup

The setup consists of a refractory tube with fine nozzle at the bottom. The refractory tube is placed over the rotating roller made up of copper.An induction heater is wounded over the refractory tube in order to heat the alloy inside the refractory tube as shown in figure.



A melt spinner consists of a **disc** made up of **copper**.Disc is rotated at a high speed - **50 m/s.**A properly **super-heated molten alloy** is **ejected under pressure** ***(helium or argon)*** through a finenozzle at the bottom of a **refractory tube** on to the spinning disc.Alloy is **melted** by **induction heating.** Ejected melt is **cooled** at a faster rate with the help of **rotating cooled copper disc.**Thus, a glassy alloy ribbon starts getting formed over the roller disc.

Properties of Metallic glasses

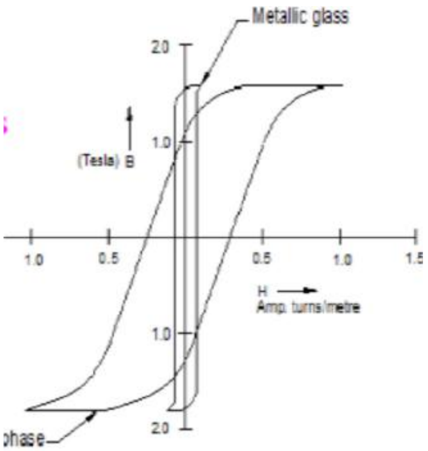
Structural Properties

(a) Metallic glasses have Tetrahedral Closely Packed (**TCP**) structure **rather than** hexagonal closely packed (**HCP**) structure.
(b) They **do not have any crystal defects** such as grain boundaries, dislocations, etc.

Mechanical (or) General Properties

(a) The metallic glasses are **very strong** in nature.
(b) They have **high corrosion resistance**.
(c) They possess **malleability**, **ductility** etc.

Magnetic Properties



(a) They exhibit high **saturation magnetisation**.
(b) Metallic glasses are **soft magnetic materials**so they can be easily magnetised & demagnetised.
(c) They have **very narrow hysteresis loop**.So the hystersis losses are almost negligible.
d) They exhibit hysteresis loss 10 very low and hence **transformer core loss is very less.**
(e) They have **high magnetic permeability** and exhibit ferromagnetism.

4. Electrical Properties
(a) Metallic glasses have **high electrical resistance (100 6-cm).**
(b) High electrical resistivity leads to **very low eddy current losses.**
(c) At **low temperature, resistivity is minimum**, below which itvaries as a logarithmic function of temperature.
(d) At **very low temperature**, **thermal expansion co-efficient isnegative.**

5. Metallic glasses are **amorphous metal** alloys which have ***no longrange atomic order***.

Applications of Metallic glasses

1. Metallic glasses are used in **tape recorder heads**, **cores of high power transformers** and **magnetic shields**, since metallic glasses possess low magnetic loss, high permeability, saturation magnetization and low coercivity.
2. They have higher workability. They can be **easily bent without breaking**. Hence these are useful in making **different kinds of springs.**
3. Metallic glasses have **high electrical resistance** with **nearly zero temperature coefficient of resistance**. Hence they are used to make **accurate standard resistances**, **computer memories**, **magnet resistance sensors** and **cryo-thermometers** (low temperature measuring thermometer).
4. Metallic glasses are very useful in the **production of veryhigh magnetic fields.**
5. Since they are **not affected by nuclear radiation**, they are used in making **containers for radioactive waste disposal.**
6. Since they have **very high corrosion resistance**, **Cr** and **P**based metallic glasses are used in **marine cables**, inner surfaceof **reactor vessels**, **orthopaedical implants** and **surgical clips**.

CERAMICS

Ceramics form an important part of materials group. Ceramics are compounds between metallic and nonmetallic elements for which the inter-atomic bonds are either ionic or predominantly ionic. The term ceramics comes from the Greek word *keramikos* which means ‘burnt stuff’. Characteristic properties of ceramics are, in fact, optimized through thermal treatments. They exhibit physical properties those are different from that of metallic materials. Thus metallic materials, ceramics, and even polymers tend to complement each other in service.

Types and properties of ceramics

Ceramics greatly differ in their basic composition. The properties of ceramic materials also vary greatly due to differences in bonding, and thus found a wide range of engineering applications. Classification of ceramics based on their specific applications and composition are two most important ways among many.

Based on their composition, ceramics are classified as:

Oxides,

Carbides,

Nitrides,

Sulfides,

Fluorides, etc.

The other important classification of ceramics is based on their application, such as:

Glasses,

Clay products,

Refractories,

Abrasives,

Cements,

Advanced ceramics.

In general, ceramic materials used for engineering applications can be divided into two groups: traditional ceramics, and the engineering ceramics. Typically, traditional ceramics are made from three basic components: clay, silica (flint) and feldspar. For example bricks, tiles and porcelain articles. However, engineering ceramics consist of highly pure compounds of aluminium oxide (Al_2O_3), silicon carbide (SiC) and silicon nitride (Si_3N_4).

Glasses: glasses are a familiar group of ceramics – containers, windows, mirrors, lenses, etc. They are non-crystalline silicates containing other oxides, usually CaO, Na_2O,

K_2O and Al_2O_3 which influence the glass properties and its color. Typical property of glasses that is important in engineering applications is its response to heating. There is no definite temperature at which the liquid transforms to a solid as with crystalline materials. A specific temperature, known as glass transition temperature or fictive temperature is defined based on viscosity above which material is named as super cooled liquid or liquid, and below it is termed as glass.

Clay products: clay is the one of most widely used ceramic raw material. It is found in great abundance and popular because of ease with which products are made. Clay products are mainly two kinds – structural products (bricks, tiles, sewer pipes) and white-wares (porcelain, chinaware, pottery, etc.).

Refractories: these are described by their capacity to withstand high temperatures without melting or decomposing; and their inertness in severe environments. Thermal insulation is also an important functionality of refractories.

Abrasive ceramics: these are used to grind, wear, or cut away other material. Thus the prime requisite for this group of materials is hardness or wear resistance in addition to high toughness. As they may also exposed to high temperatures, they need to exhibit some refractoriness. Diamond, silicon carbide, tungsten carbide, silica sand, aluminium oxide / corundum are some typical examples of abrasive ceramic materials.

Cements: cement, plaster of paris and lime come under this group of ceramics. The characteristic property of these materials is that when they are mixed with water, they form slurry which sets subsequently and hardens finally. Thus it is possible to form virtually any shape. They are also used as bonding phase, for example between construction bricks.

Advanced ceramics: these are newly developed and manufactured in limited range for specific applications. Usually their electrical, magnetic and optical properties and combination of properties are exploited. Typical applications: heat engines, ceramic armors, electronic packaging, etc.

Some typical ceramics and respective applications are as follows:

Aluminium oxide / Alumina (Al_2O_3): it is one of most commonly used ceramic material. It is used in many applications such as to contain molten metal, where material is operated at very high temperatures under heavy loads, as insulators in spark plugs, and in some unique applications such as dental and medical use. Chromium doped alumina is used for making lasers.

Aluminium nitride (AlN): because of its typical properties such as good electrical insulation but high thermal conductivity, it is used in many electronic applications such as in electrical circuits operating at a high frequency. It is also suitable for integrated circuits. Other electronic ceramics include – barium titanate ($BaTiO_3$) and Cordierite ($2MgO$-$2Al_2O_3$-$5SiO_2$).

Diamond (C): it is the hardest material known to available in nature. It has many applications such as industrial abrasives, cutting tools, abrasion resistant coatings, etc. it is, of course, also used in jewelry.

Lead zirconium titanate (PZT): it is the most widely used piezoelectric material, and is used as gas igniters, ultrasound imaging, in underwater detectors.

Silica (SiO_2): is an essential ingredient in many engineering ceramics, thus is the most widely used ceramic material. Silica-based materials are used in thermal insulation, abrasives, laboratory glassware, etc. it also found application in communications media as integral part of optical fibers. Fine particles of silica are used in tires, paints, etc.

Silicon carbide (SiC): it is known as one of best ceramic material for very high temperature applications. It is used as coatings on other material for protection from extreme temperatures. It is also used as abrasive material. It is used as reinforcement in many metallic and ceramic based composites. It is a semiconductor and often used in high temperature electronics. Silicon nitride (Si_3N_4) has properties similar to those of SiC but is somewhat lower, and found applications in such as automotive and gas turbine engines.

Titanium oxide (TiO_2): it is mostly found as pigment in paints. It also forms part of certain glass ceramics. It is used to making other ceramics like $BaTiO_3$.

Titanium boride (TiB_2): it exhibits great toughness properties and hence found applications in armor production. It is also a good conductor of both electricity and heat.

Uranium oxide (UO_2): it is mainly used as nuclear reactor fuel. It has exceptional dimensional stability because its crystal structure can accommodate the products of fission process.

Yttrium aluminium garnet (YAG, $Y_3Al_5O_{12}$): it has main application in lasers (Nd-YAG lasers).

Zirconia (ZrO_2): it is also used in producing many other ceramic materials. It is also used in making oxygen gas sensors, as additive in many electronic ceramics. Its single crystals are part of jewelry.

Fabrication and processing of ceramics

Ceramics melt at high temperatures and they exhibit a brittle behavior under tension. As a result, the conventional melting, casting and thermo-mechanical processing routes are not suitable to process the polycrystalline ceramics. Inorganic glasses, though, make use of lower melting temperatures due to formation of eutectics. Hence, most ceramic products are made from ceramic powders through powder processing starting with ceramic powders. The powder processing of ceramics is very close to that of metals, powder metallurgy. However there is an important consideration in ceramic-forming that is more prominent than in metal forming: it is dimensional tolerance. Post forming shrinkage is much higher in ceramics processing because of the large differential between the final density and the as-formed density.

Glasses, however, are produced by heating the raw materials to an elevated temperature above which melting occurs. Most commercial glasses are of the silica-soda-lime variety, where silica is supplied in form of common quartz sand, soda (Na_2O) in form of soda ash (Na_2CO_3) while the lime (CaO) is supplied in form of limestone ($CaCO_3$). Different forming methods- pressing, blowing, drawing and fiber forming- are widely in practice to fabricate glass products. Thick glass objects such as plates and dishes are produced by pressing, while the blowing is used to produce objects like jars, bottles and light bulbs. Drawing is used to form long objects like tubes, rods, fibers, whiskers etc. The pressing and blowing process is shown in figure

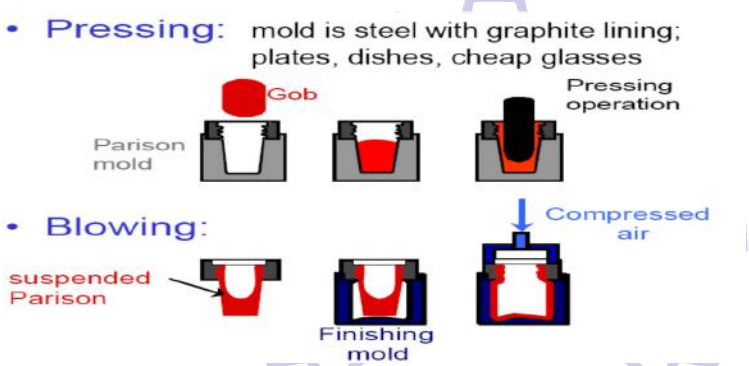


Figure : *Schematic diagram of pressing and blowing processes*

Extrusion and injection molding techniques are used to make products like tubes, bricks, tiles etc. The basis for **extrusion** process is a viscous mixture of ceramic particles, binder and other additives, which is fed through an extruder where a continuous shape of green ceramic is produced. The product is cut to required lengths and then dried and sintered. **Injection molding** of ceramics is similar to that of polymers. Ceramic powder is mixed with a plasticizer, a thermoplastic polymer, and additives. Then the mixture is injected into a die with use of an extruder. The polymer is then burnt off and the rest of the ceramic shape is sintered at suitable high temperatures. Ceramic injection molding is suitable for producing complex shapes. Figure shows schematically the injection molding process

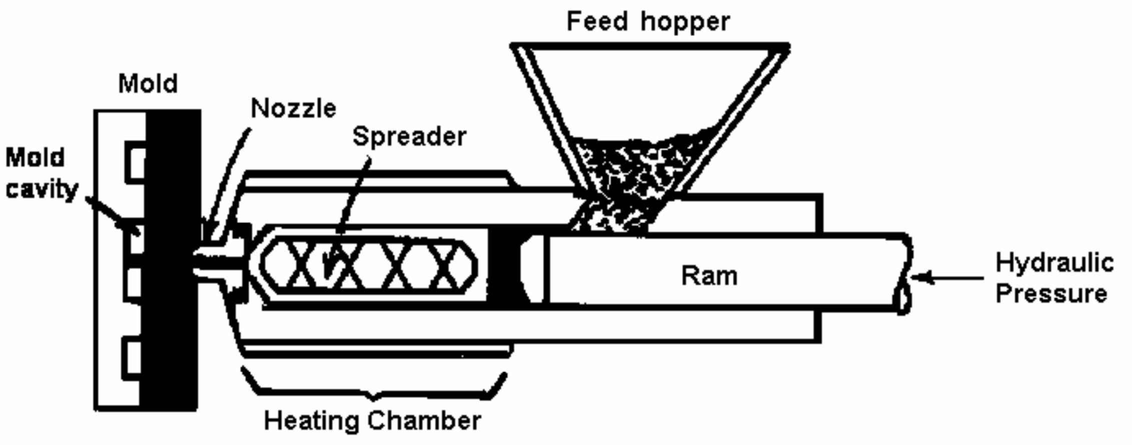


Figure Schematic diagram of Injection molding

Sintering is the firing process applied to green ceramics to increase its strength. Sintering is carried out below the melting temperature thus no liquid phase presents during sintering. However, for sintering to take place, the temperature must generally be maintained above one-half the absolute melting point of the material. During sintering, the green ceramic product shrinks and experiences a reduction in porosity. This leads to an improvement in its mechanical integrity. These changes involve different mass transport mechanisms that cause coalescence of powder particles into a more dense mass. With sintering, the grain boundary and bulk atomic diffusion contribute to densification, surface diffusion and evaporation condensation can cause grain growth, but do not cause densification. After pressing, ceramic particles touch one another. During initial stages of sintering, necks form along the contact regions between adjacent particles thus every interstice between particles becomes a pore. The pore channels in the compact grow in size, resulting in a significant increase in strength. With increase in sintering time, pores become smaller in size. The driving force for sintering process is the reduction in total particle surface area, and thus the reduction in total surface energy. During sintering, composition, impurity control and oxidation protection are provided by the use of vacuum conditions or inert gas atmospheres.

Shape memory Alloys

An **alloy** is a **partial** or **complete** solid solution of**one** or **more** elements in a metallic matrix. ***Complete solid solution*** alloys give **single solid phase**microstructure.

Partial solid solutions give **two or more phases** which are **homogeneous** in distribution depending on **heat treatment.**
Alloying one metal with other metal(s) or non metal(s) often **enhances** its properties.

Physical properties

such as ***density***, ***reactivity***, ***young's modulus***, and ***electrical*** and ***thermal conductivity*** of an alloy may **not differ** greatly from those of its elements.

Engineering properties

such as ***tensile strength*** and ***shear strength*** may be substantially **different** from those of the constituent materials.

Steel is a **metal alloy** whose major component is **iron** with **carbon** content between 0.02% and 2.14% by mass. For example, **steel** is **stronger** than **iron**, its primary element.
Brass is an alloy made from **copper** and **zinc**.
Bronze used for ***bearings***, ***statues***, ***ornaments*** and ***church bells***, is an alloy of **copper** and **tin**.
1. Unlike pure metals, most alloys **do not** have a **single melting point**.
2. Instead, they have a **melting range** in which the material is a mixture of **solid** and **liquid** phases.

A metal that "remembers" its geometry

Shape Memory Alloy (SMA),Smart Metal (or) Memory Alloy, Smart Metal Intelligent Materials (or) Smart Alloy, Muscle Wire (or) Active Materials

Shape Memory Alloys (SMAs)

Shape memory alloys are special type of alloys which **after being deformed** can **remember** and **recover** their**original shape** when subjected to the appropriate **thermal** procedure (Heating / Cooling).

The ability of the metallic alloys to retain their original shape when heating/cooling.

Three main types of shape memory alloys

1. **C**opper-**Al**uminium-**Ni**ckel (AlNiCo)
2. **C**opper-**Z**inc-**Al**uminum-**Ni**ckel and
3. **Ni**ckel-**Ti**tanium (NiTi) alloys.

SMA's can also be used by alloying **Zinc**, **Copper**, **Gold**, **Manganese** and **Iron**.

Examples of SMA's
a. Au - Cd alloy b. Ti - Ni alloy c. Mn - Cu alloy
d. Ni - Mn - Ga alloy e. Cu - Al - Ni alloy.

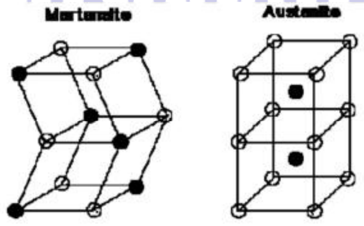
Transformation Temperature

Shape recovery process occurs not at a single temperature, rather it occurs **over a range of temperature. (60-1450 K)** The **range of temperature** at which the SMA **switches from new shape** to **its original shape** is called **Transformation Temperature (or) Memory Transfer Temperature.**

Below **Tt** , SMA can be **bent into various shapes**.
Above **Tt** , SMA **returns to its original shape**.
This ***change in shape*** was mainly caused due to the **change in crystal structure** (phase) within the materials, **due to the rearrangement of atoms** within itself.

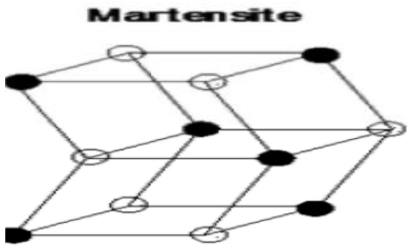
Phases of SMA

In general the SMA has **two phases** (crystal structures) viz.,
(i) **Martensite** and
(ii) **Austenite**

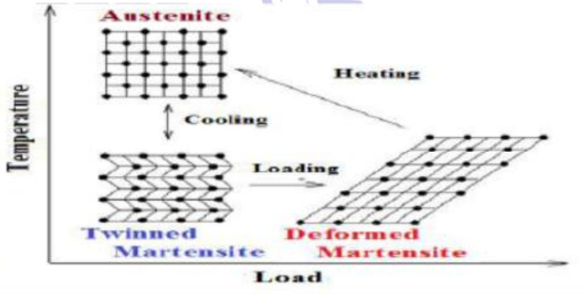


Martensite, named after the German metallurgist **Adolf Martens** (1850–1914),

Solid crystalline structure most commonly **refers** to a **very hard form** of **steel crystalline structure.**



Martensite is an interstitial **super solution** of **carbon** in **α-iron** and it crystallizes into **twinned structure**.
It has **platelet** structure.
Martensite is the relatively **soft** and **easily deformed phase** of shape memory alloys which exists at **lower temperatures**.

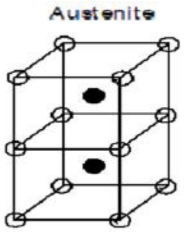


Martensite structure have two forms
a) **Twinned** martensite*before* loading and
b) **Deformed** martensite *after* loading.

Austenite

Austenite (or ***gamma phase iron***) is a metallic **non-magnetic allotrope of iron** or a ***solid solution*** of ***iron***, with an alloying element. ***solid solution*** of ***iron***

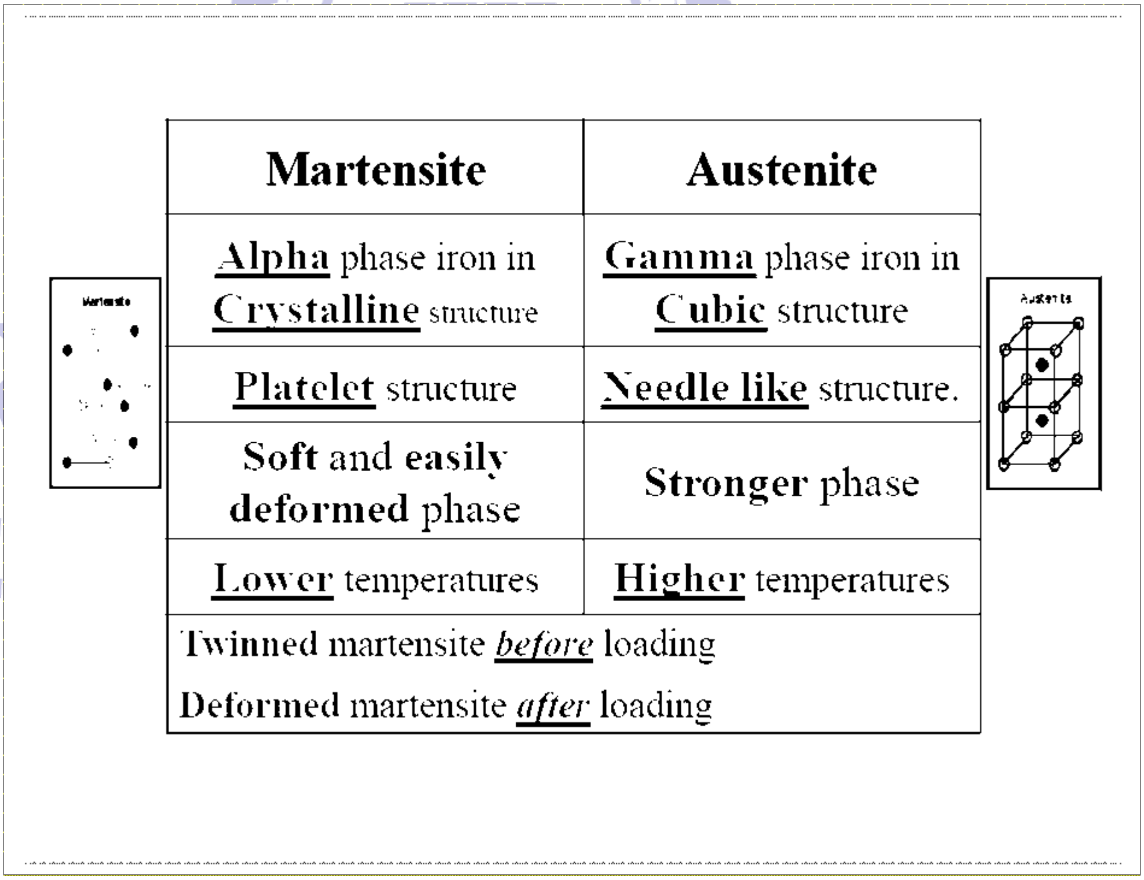
It is named after **Sir William Chandler Roberts-Austen** (1843-1902).



Austenite is the **solid solution** of **carbon** and other alloying elements in **g-iron** and it crystallizes into **cubic structure**.

It has **needle like** structure.

Austenite is the **stronger** phase of shape memory alloys which occurs at **higher temperatures**.



Martensite	Austenite
Alpha phase iron in **Crystalline** structure	**Gamma** phase iron in **Cubic** structure
Platelet structure	**Needle like** structure.
Soft and **easily deformed** phase	**Stronger** phase
Lower temperatures	**Higher** temperatures
Twinned martensite ***before*** loading Deformed martensite ***after*** loading	

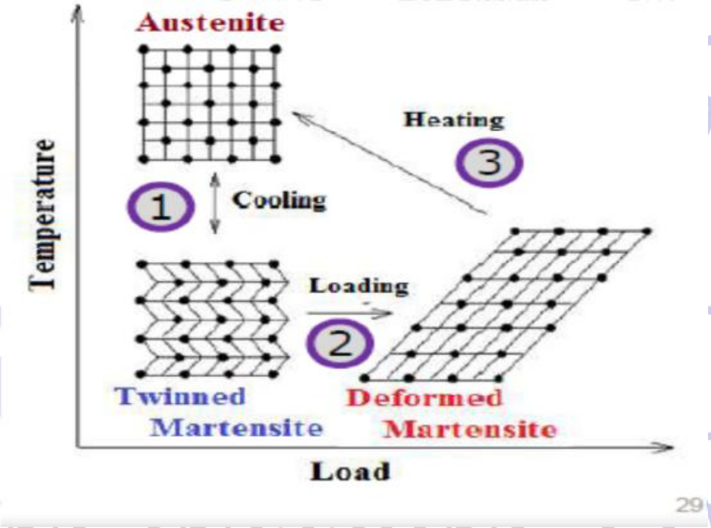
Characteristics of SMA

SMA's are metals which exhibit two unique properties
1. **Shape Memory Effect *with change in temperature***

2. **Pseudo elasticity (or) Super elasticity** ***without change in temperature***

Shape Memory Effect

The phenomenon in which the shape memory alloy apparently **deformed** at **lower temp** and **returns** to its original shape (former shape) when heated to **higher temp**". When **temperature** is **decreased**, phase **transformation** take place from **austenite** to **twinned martensite.** i.e., a micro constituent transformation takes place from the **Austenite** to **Martensite.**

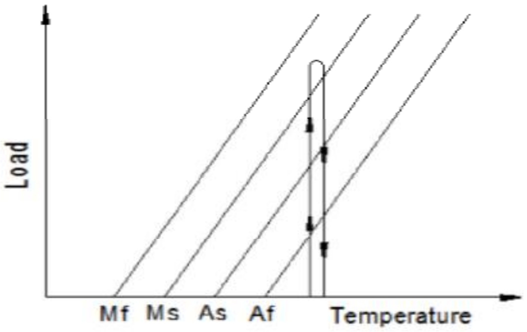


During this state the ***twinned martensite*** phase will have **same size** as that of ***austenite phase***. When **load** is applied to the ***twinned martensite***, it goes to **deformed martensite** phase. When the material is **heated** it will go from ***deformed martensite*** to **austenite form** and the cycle continues.

Pseudo-elasticity (or) Super Elasticity

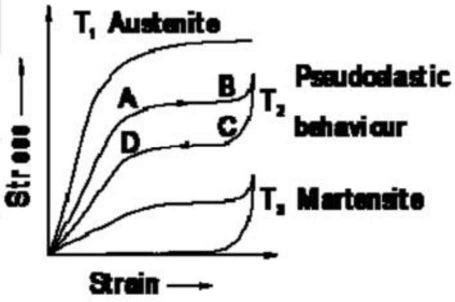
a) Pseudo-elasticity occurs in shape memory alloys when the alloy is **completely** composed of **austenite** (temperature is greater than Af).

b) Unlike the shape memory effect,pseudo-elasticity ***occurs without a change in temperature.***



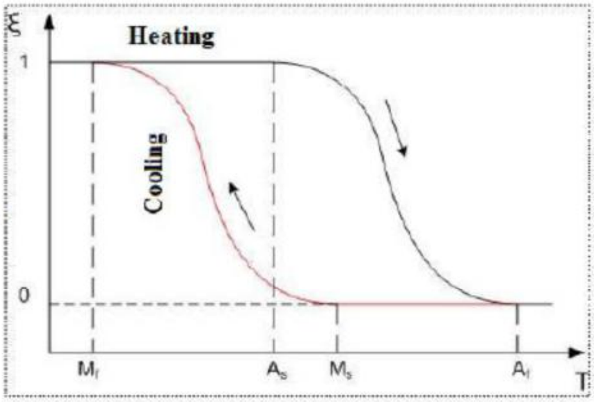
Pseudo-elasticity

The **martensitic** phase is generated by **stressing** the metal in the **austenitic** state and this martensite phase is capable of **large strains**. With the **removal** of the load, the **martensite transforms** back into the **austenite** phase and resumes its original shape.(Process similar to pressing a rubber or spring).



Hysteresis

On heating - Transform – Martensite to Austenite. The **difference** between the **transition temperatures** upon **heating and cooling**" is called ***Hysteresis.*** "The difference between the temperature at which the material is **50% transformed** to **austenite upon heating** and **50% transformed** to **martensite upon cooling**". Difference can be up to 20- 30ºC.



Effects of SMA

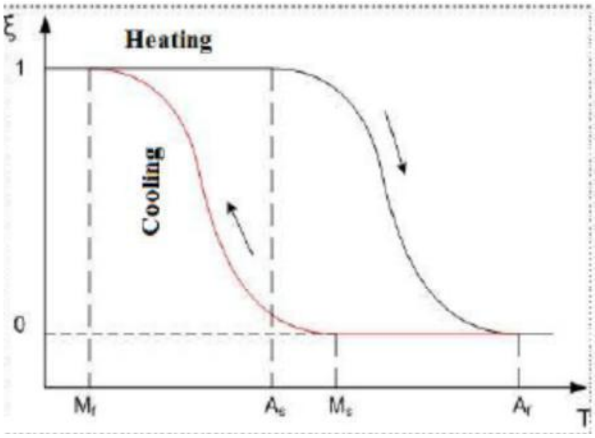
(i) **One-way** shape memory alloy

(ii) **Two-way** shape memory alloy

(i) One - way SMA :

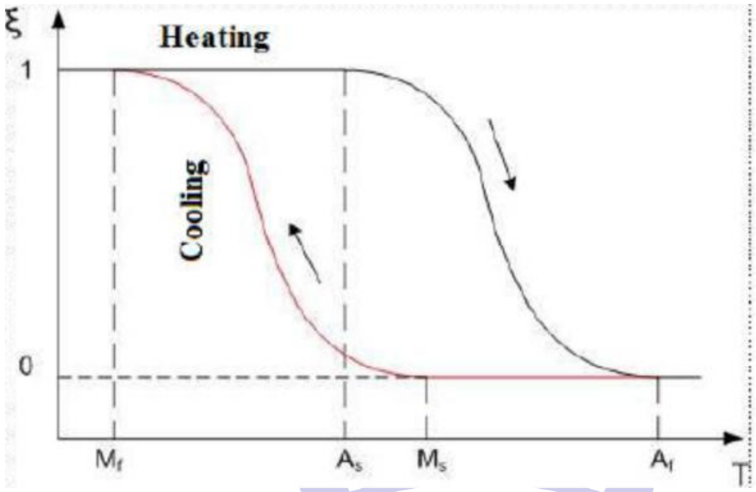
When the material is **cooled** belowthe **martensite ends** (Mf) temperature. Then there exist some minor change and will remain in martensite form alone.

Thus, though there is some change in its temperature, the SMA remains in the same phase and this type of material *is called* ***one way shape memory alloy***.



(ii) Two - way SMA :

If the **temperature** is **increased** then the **martensite** becomes **austenite** and if the **temperature** is **decreased** it **reverses** its state.



Applications of SMAs

1) **Fire safety** valve
2) Antenna **wires**
3) **Toys** and novelties
4) **Eye glass frames**
5) Coffee pot **thermostats**
6) Helicopter **blades**
7) **Blood - clot filter**
8) Cryofit hydraulic couplings
9) Circuit **edge connector**
10) Correct the **irregularities** in **teeth**
11) Artificial **hip-joints, bone-**11**plates**

Advantages of SMA

1 .Simplicity, compactness and **safety mechanism.**

2. **Bio – compatibility**.
3. Diverse fields of application, clean, silent, spark free working condition .
4. Good mechanical properties. (strong, corrosion resistant)

Disadvantages of shape memory alloys

1. Degradation **poor fatigue** properties.
2. **Expensive**.
3. **Low energy** efficiency.
4. **Limited bandwidth** due to heating and cooling restrictions.

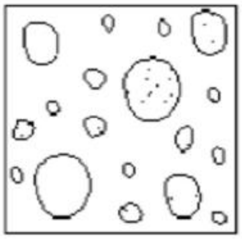
NANO PHASE MATERIALS

Nano science is the study of the fundamental principles of **molecules** and **structures** with atleast one dimensions in the range about **10–9 m to 10–7 m** (1 to 100 nm).
Atoms are extremely small and the diameter of a single atoms can vary from 0.1 to 0.5 nanometers depending on the type of elements (nanometer is 10–9 m).

Nanotechnology is **largely concerned with solid phases** because the molecules (or) atoms do not move away from each other. All materials are **composed of grains**, which in turn comprise may atoms Nanomaterials when in powder form (called nanopowder) have grain sizes in the order of 1 - 100 nm.ex : **ZnO, Cu-Fe alloy, Ni, Pd, Pt**, etc.

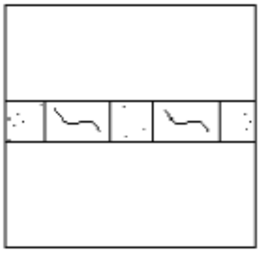
In nanomaterials the majority of the atoms are **located on the surface of the particles** and hence the atoms are of a different environment. Nanomaterials have **increased surface area** of the substance with high surface areas have **enhanced *chemical***, ***mechanical optical*** and ***magnetic*** properties. Nanotechnology is a field of applied science focused on the **design**, **synthesis**, **characterization** and **application** of materials and devices on the nanoscale.

*Classification based on the **number of dimensions** lie with in the nanometer range.*
(1) Zero dimensional nano structure (0D)
Ex : atoms



(2) One dimensional nano structure (1D)
Ex : atom clusters
Multilayered material with layer of thickness in the nanometer range - **1D**.

(3) Two dimensional nano structure (2D)
Ex : Nano tube.
Layers in the nanometer thickness range - **2D**.



(4) Three dimensional nano structure (3D)

Ex : Quantum well.

Material with three dimensional equiaxed nano size grain.

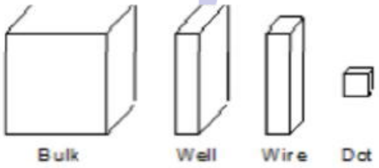
Quantum wells, Quantum wires and Quantum dots

When size of a material - reduced -bulk or macroscopic size - very small size

Properties remain same

Size drops below 100 nm **Drastic changes in properties can occur**.

If **1 D- reduced** - nanorange -
while the ***other two dimensions*** **remain large** – resulting structure.



If **2 D** - **reduced** - nanorange - ***one*** **remains large** – resulting structure.
Size reduction in which all three dimensions leads to low nanometer.

FABRICATION METHOD

BOTTOM UP

It results due to **building blocks** such as atoms and molecules and **assemble them** into larger nanostructured material.

TOP DOWN

It results due to **breaking down** of large pieces of bulk material to generate the required form.

Top-down approach

a. Milling
b. Lithographics
c. Machining

Bottom - up approach

1. Vapor phase deposition methods
a. **Chemical vapor deposition**
b. Physical vapor deposition
2. .**Plasma assisted deposition process**
3. Molecular beam epitaxy (MBE)
4. Metal organic vapor phase epitaxy (MOVPE)
5. Liquid phase processes
a. Colloidal method
b. **Sol-gel method**

Top-down approach

Top-down processes starts with large scale object and **gradually reduces** its dimensions. The top-down approaches are **simpler**.Methods used to produce nanostructured materials under top-down approach are given below.

a. Milling
b. Lithographics
c. Machiningpproach

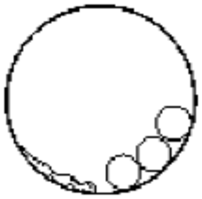
High Energy Ball Milling

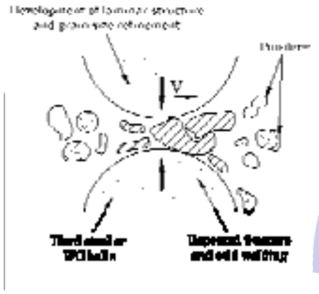
1) Itis also known as ***Mechanical alloying*** *or* ***Mechanical attrition.***
2) It is a **solid state** process.
3) High energy ball milling can induce **structural changes** and **chemical reactions** at **room temperature.**

Procedure:

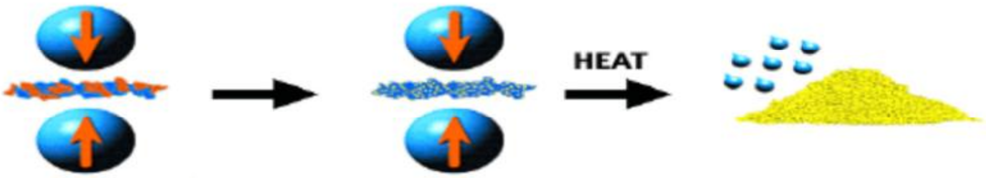
It consists of **stainless steel rotating drum** with **hard steel** or **tungsten carbide balls** inside it.

The container is purged and **argon** is introduced to **prevent** unwanted reaction such as **oxidation**. Milling is carried out at room temperature for upto **150 hours.** Powder materials are **crushed mechanically** in the **rotating drum** by the hard balls. This repeated deformation can cause **large reductions in grain size** in the powder particles.





High energy ball milling is used for the production of
a. ***Nanocrystalline*** *materials b.* ***Nanoparticles***
c. ***Nanocomposites*** *d.* ***Nanotubes*** *e.* ***Nanorods*** *and f.* ***Nanowires***



This technique can be used at a **large scale level** and hence is of much **industrial interest**. Controlled ball milling technique has a large range of applications in processing nanomaterials such as **opening of caped nanotubes**, **preparing fine catalyst** particles and **improving hydrogen storage** in nanotubes.

Ball mill acts as a low temp Chemical reactions occur at Reaction product is heat
Chemical reactor, reaction nanoscale. Low temp enables treated. Solid phase chemistry
process results from local controlled nano particle prevents particles from
heat and pressure at formation. agglomeration. contact surface.

Bottom - up approach

Atoms, molecules and even nanoparticles themselves can be ***used*** as the **building blocks** for the **creation** of larger nanostructure with required properties.
By ***changing the size*** of the building blocks and controlling their assembly and arrangement it is **possible to change the properties** of the nanostructured material.
Synthesis, collection, consolidation and arrangement of individual atoms and molecules into the larger nanostructure is carried out by a sequence of chemical reactions **controlled by**

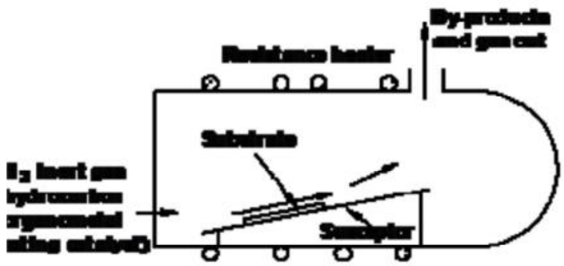
catalysts. This is a very ***powerful approach*** of creating identical structures with **atomic precision**.

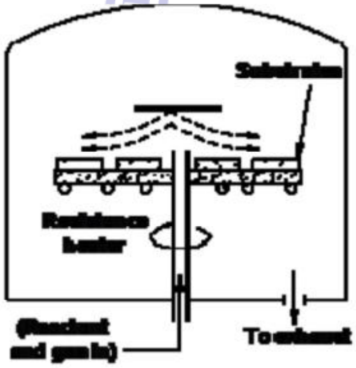
1. Vapor Phase Deposition methods (CVD)
2. Plasma assisted deposition process
3. Molecular Beam Epitaxy (MBE)
4. Metalorganic vapour phase epitaxy
5. Liquid phase processes
a. Colloidal method b. Sol-gel method

Bottom - Up approach

Chemical Vapor Deposition (CVD)

CVD involves the **flow of a gas** with **diffused reactants over a hot substrate surface.** Gas that carries the reactants is called the ***carrier gas.*** While the gas flows over the hot solid surface, the **heat energy provokes chemical reactions of the reactants** that **form film during** and **after** the reactions. By product of the chemical reactions are then **vented**. Thin film of **desired composition** can thus be created over the surface of the substrate. **Resistance heaters** either surround the chamber or **lie directly under** the susceptor that holds the substrates.



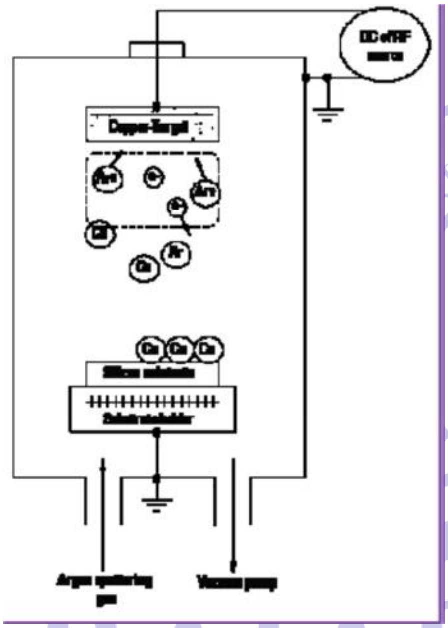


In CVD method carbon nanotubes are grown from the **decomposition of hydrocarbons at temperature range of 500 to 1200oC.** They are grown on **substrates** such as **carbon, quartz and silicon** or on floating **fine catalyst** particles like **CO, Fe, Ni** from **hydrocarbons** such as **benzene, xylene or acetylene. Growth of nanostructures** can occur either in the **heating zone before or after the heating zone.** The growth process takes about **30 minutes**. The flow of H2 gas is maintained at 200 ml/minutes. Inert gas is used to cool the reactor.

PLASMA ARCING PROCESS

Sputtering is a process in which ***energetic ions knock*** atoms or molecules ***from a target*** that act as one ***electrode*** and subsequently ***deposit*** them on a ***substrate*** that is acting as an ***another electrode***. The **material to be deposited** serves as a **cathode (target)** and the **substrate on which the material be deposited to** serve as an **anode**. The target and the substrate **face each other** in the sputtering chamber. After evacuation of the chamber an **inert gas argon** is introduced and **serves as the medium** in which the **electrical discharge is initiated** and **maintained**. ***The use of plasma i.e., ionised gas during vapour deposition is found to yield high purity final material relative to the PVD and CVD techniques.***

When **dc voltage** of few kilovolts is applied and adjusted between the electrodes **a visible glow discharge** is initiated and maintained. Now the **free electrons** will be **accelerated** by the **electric field** and gain **sufficient energy** to **ionise argon atoms**. Resulting **positive ions Ar+** in the discharge **strike** the **cathode** and **physically eject or sputter target atoms** through momentum transfer to them. These atoms **pass through the discharge** and **deposit on the substrate** with growing film.In addition to the growth species other particles like **neutral atoms**, **electrons** and **negative ions** under electric field **will also bombard** and **interact** with the surface of the substrate or grown film. For the deposition of insulating films an **alternate electric field of frequency 13.56 MHz** is applied to **produce plasma** between the electrodes.



Multiple targets can be **rotated** so as to produce a multilayered coating on the substrate.The sputtered film consists of **smaller grains with better adhesion** to the substrate.By **introducing a magnetic field** near the target in the sputtering process, the **deposition rate** can be **increased to 1 mm / minute** and also it **prevents** the **substrate heating due to secondary electron impingement** from the target.Such sputtering process with **process with magnetic field** is called ***magnetron sputtering.*** **Reactive gases** have also been introduced into the chamber to form compound films which are known as ***reactive sputtering.***

There are different types plasma-assisted deposition techniques.

a). DC sputtering, b). RF sputtering c). Reactive sputtering.

d). DC magnetron sputtering e). RF magnetron sputtering.

Sol-gel Method

It is a **versatile industrial approach** for fabricating nanomaterials.

It is a **solution phase synthetic route** to produce **highly pure** ***organic*** or ***inorganic*** materials that have homogeneous particle and pore sizes as well as densities. This method affords **easy control over the stoichiometry and homogeneity** that conventional methods lack.

This technique allows us to **change the composition** and **structure** of **materials** on the **nanometer scale.** Its benefits include the convenience of **low-temperature preparation** using general and **inexpensive laboratory equipment**. One of the important features of the technique is its ability to produce materials in different forms, such as **powders**, **films**, **fibres** of **nanosize** and **free standing pieces** of **materials** called **monoliths**. Scientists have used this technique to produce the **world's lightest materials and some of the toughest ceramics.**

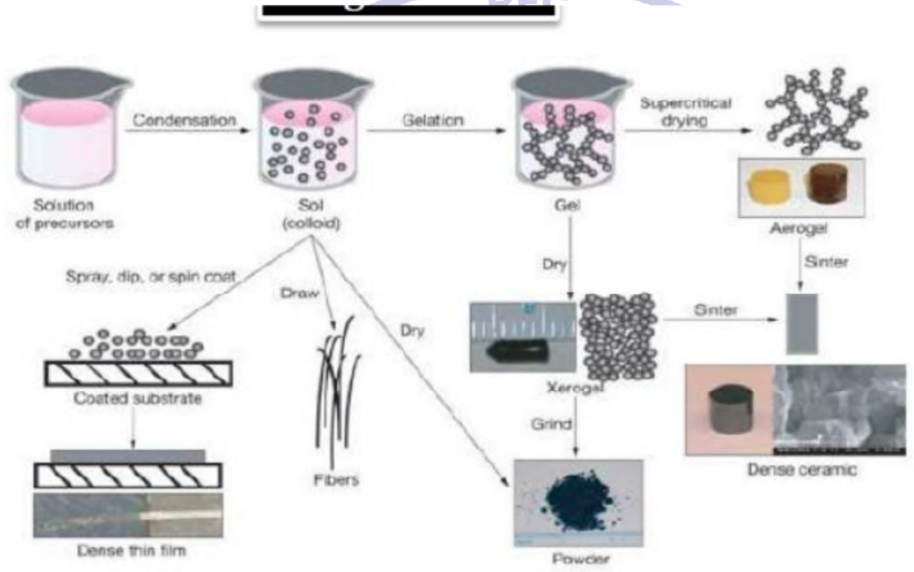
This method is based on the **phase transformation** of a solution obtained from **metallic alkoxides** or **organo-metallic precursors**. Solution containing particles in suspension is **polymerized** at **low temperature** to form a **wet gel**. Wet gel is then **densified** through **thermal annealing** to get the products like a **glass**, **polycrystals** or a **dry gel**. Typically this involves a **hydrolysis reaction followed by condensation and polymerization.** For example

Tetraethylorthosilicate (TEOS) (Si(OC2H5)4) + ethanol (C2H5OH) SiO2 + other products

Polymer gel so formed is a **3 D skelton** surrounding **interconnected pores** and this can be **dried and shrunk to form a rigid solid form. Transformation to gel** is achieved by **changing the pH** or the **concentration** of the solution. **Super critical drying process removes** the **liquid phase** from the gel and **produces a low-density 3D porus material** called **AEROGEL**. Aerogels **densities** are typically between **1 - 20%** that of the **bulk** material. When the gel is **dried slowly** in a **fluid evaporation process**, the gels **original network collapses**, which creates a high density material known as a **XEROGEL**.

Xerogel **densities** can be between **30 - 80%**that of the **bulk material**. The method starts with a solution consisting of **metal compounds** such as **metal alkoxides** and **acetylacetonates** as **source of oxides**, **water** as **hydrolysis** agent, **alcohol** as **solvent** and **acid** or **base catalyst**.

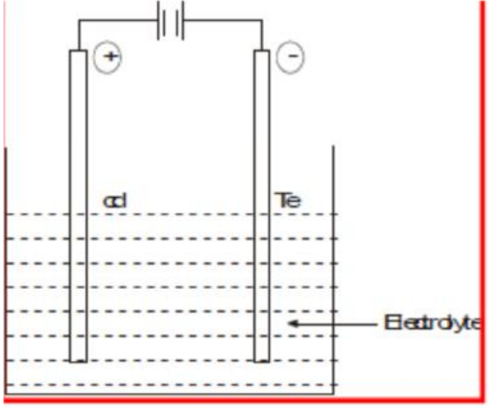
Tetra ethyl ortho silicate (TEOS) (Si(OC2H5)4)+ ethanol (C2H5OH) SiO2 + other products



Electrodeposition

It is the process in which *chemical reactions occur in a electrolyte solution by the* ***application of voltage.*** *This process is known as "****electroplating****". Electro deposition process requires an* ***electrically conducting substrate.*** Synthesized materials are ***mechanically***

strong, uniform and strong. In the electroplating process the **substrate** is placed in a ***liquid solution (electrolyte)***. When an **electrical potential** is applied **between** a ***conducting area on the substrate*** and a ***counter electrode*** (usually platinum) in the liquid, a chemical process takes place resulting in the **formation of a layer of material on the substrate** and usually some gas generation at the opposite electrode.



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Electrodeposition is basically classified into
a) **Anodic** electrodeposition and
b) **Cathodic** electrodeposition.

In an **Anodic** Process, a ***metal anode*** is electrochemically oxidized in the ***presence of other ions in solution***, which then react together and deposit on the anode.
Ex : Cd----- Cd2+ + 2e–
Cd2+ + Te2–----- Cd Te

In a **Cathodic** process components are deposited onto the cathode from ***solution precursors***.
Ex : Cd2+ + 2e–--- Cd
HTeO2+ + 4e– + 3H+------- Te + 2 H2O
Cd 2+ + Te2– ------Cd Te

Properties of Nano Particles

Physical properties

i. Since the size of the particle is very less - ***inter particle spacing*** is ***very less*** innanomaterials.
ii. Because of its very less size, these nano materials ***cannot be further divided*** into small particles and it ***does not have any dislocation*** in it. Thus we can say that they have ***high strength and super hardness.***
iii. The ***melting point*** of nanomaterials will be ***very less***.

Mechanical properties

i. The ***hardness*** of nano phase materials is due to the phase transformation, stress relief, density and grain boundaries.
ii. They exhibit ***super plastic*** behaviour.

Magnetic properties

i. In nano-materials a **large number of atoms** will be present at the**surface**. These atoms will have ***less-co-ordination number*** and hence posses ***local magnetic moment with in themselves***.
ii. Due to large magnetic moment these nano-materials exhibits ***spontaneous magnetisation at smaller sizes***.
iii. Ferro-magnetic and anti ferro magnetic multilayer nano-materials has
GMR (Giant Magneto Resistance) effect.

iv. The nanomaterials ***shows variation*** in their **magnetic property**, when ***they change*** from ***bulk state*** to ***cluster*** (nano particle) state.

Materials	Bulk state	Nano phase state
1 Iron, Ni, Cobalt	**Ferro magnetic**	**Super para magnetic**
2 Na, K	**Ferro magnetic**	**Ferro magnetic**
3 Cr	**Anti ferromagnetic**	**Frustrated Para magnetic**.

Electrical properties

i. The **energy bands** in these materials will be ***very narrow***.
ii. The **ionization potential** is found to be **higher**.
iii. When the nanomaterials are ***prepared from bulk materials***, they have ***more localized molecular bands***.
iv. Nano-materials are capable of **storing hydrogen** atoms.

APPLICATIONS OF NANO MATERIALS

(i) Mechanical Engineering

a) Since they are **stronger**, **lighter** etc., they are used to ***make hard metals.***
b) Smart magnetic fluids are used in **vaccum seals**, **magnetic separators** etc.,
c) Used in **Giant Magneto Resistance (GMR)** spin valves.
d) **Nano-MEMS** (Micro - Electro Mechanical Systems) are used in ***ICs***, ***Optical switches***, ***Pressure sensors***, ***Mass sensors*** etc.

(ii) Electrical, Electronics and Communication Engineering

a) ***Orderly assembled*** nanomaterials are used as **quantum electronic devices**and **photonic crystals**.
b) They are used as **sensing elements**.
c) Especially the **molecular nanomaterials** are used to design the ***robots***, ***assemblers*** etc.
c) They are used in **energy storage devices** such as ***hydrogen storage devices, magnetic refrigeration*** and in ***ionic batteries***.
d) **Dispersed nanomaterials** are used in ***magnetic recording devices***, ***rocket propellant, solar cells, fuel cells,*** etc.
e) Used to **design nano-robots**, which are used to ***remove*** the **damaged cancer cells** and also to ***modify*** the **neutron network** in human body.

(iii) Computer Science Engineering and IT

a) Nanomaterials are used to make **CD's** and **Semiconductor Laser**.

b) They are used as to **store information in smaller chips.**
c) They are used in **mobiles, Laptops, etc.,**
c) They are used in **Optical computers.**
d) **Nan-dimensional photonic crystals** and **Quantum electronic devices** plays a vital role in computer industry.

(iv) Bio-Medical and Chemical Engineering

a) Bio-Sensitive nanoparticles are used in the production of **DNA Chips, Bio-sensors**, etc.,
b) Nano structed ceramic materials are used in **synthetic bones.**
c) Nano metallic colloids are used as **film precursors. Catalyst, Electrodes Solar Cells Fuel Cells.**
c) They are used as in & d) Nano materials are used as **adsorbents, self-cleaning glass, fuel additives, drugs, ferro fluids.**

COMPOSITES

Modern engineering materials are **composite materials**, which are

prepared by **grouping** one kind of material with the other.
1. Metal mixed with polymer.
2. Ceramic mixed with metals.
It was found that the resultant materials with **peculiar properties** which varies with respect to the **size**, **shape** and the **nature** of **mixture**.

Composite materials have changed the world of materials revealing materials which are different from common heterogeneous materials. A composite material is a structural material that consists of two or more combined constituents which are combined at macroscopic level and are not soluble in each other. It should be understood that the aforesaid composite material is not the by-product of any chemical reaction between two or more of its constituents.

E.g :- Natural composites exist in both animals and plants. Wood is a composite – made from cellulose fibres (a polymer) held in lignin matrix. The two weak substances lignin and cellulose together form a much stronger composite.

Composites are a combination of two materials in which one of the materials is called the reinforcing phase embedded in the other material called the matrix phase. The reinforcing phase material may be in the form of fibers, particles, or flakes (e.g. Glass fibers). The matrix phase materials are generally continuous (e.g. Epoxy resin).

a. Role of Reinforcements:

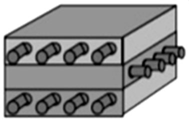
Reinforcements give high strength, stiffness and other improved mechanical properties to the composites. Also their contribution to other properties such as the co-efficient of thermal expansion, conductivity etc., is remarkable.

b. Role of Matrices:

Even though having inferior properties than that of reinforcements, its physical presence is must;

- To give shape to the composite part.
- To keep the fibers in place.
- To transfer stresses to the fibers.
- To protect the reinforcement from the environment, such as chemicals & moisture.
- To protect the surface of the fibers from mechanical degradation.
- To act as shielding from damage due to handling.

Composition of composites

Fibre/Filament Reinforcement	**Matrix**	**Composite**
		= 
• High strength • High stiffness	• Good shear properties	• High strength • High stiffness

• Low density	• Low density	• Good shear properties • Low density

Components of composite materials

Matrix	Reinforcement material	Properties
Polymer	Epoxides, polyesters, nylons, etc	Good abrasion resistance, High tensile strength, High stiffness
Metal	Metal fibers, ceramic, carbon, glass	Electric resistance to temperature, increased thermal stability
Ceramic	Particles and metallic fibers and ceramics	Chemical and thermal resistance to temperature.
Glass	Glass and ceramic particles	Mechanical strength and chemical resistance to temperature. Increased thermal stability
Organic	Carbon, glass and organic fibers	Mechanical strength to high temperature. chemical and electrical, and erosion resistance, flexibility and thermal stability

Advantages of composite

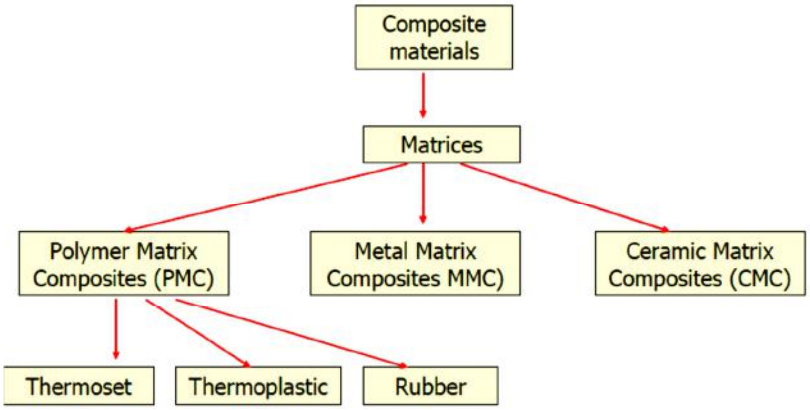
Composites can be very strong and stiff, yet very light in weight, so ratios of strength-to-weight and stiffness-to-weight are several times greater than steel or aluminum

- Higher specific strength than metals, non-metals, and even alloys.
- Lower specific gravity in general.
- Improved stiffness of the material.
- Composite maintain their weight even at high temperatures.
- Toughness is improved.
- Fabrication or production is cheaper.
- Creep and fatigue strength is better.
- Controlled Electrical conductivity is possible.
- Corrosion and oxidation resistance.

Applications of Composite Material

- In automobile industries (e.g. Steel &Aluminium body)
- Marine applications like shafts, hulls, spars (for racing boats)
- Aeronautical application like components of rockets, aircrafts (business and military), missiles etc.
- Communication antennae, electronic circuit boards (e.g. PCB, breadboard)
- Safety equipment like ballistic protection and airbags of cars.

CLASSIFICATION BASED ON MATRICES



Polymer-Matrix Composites (PMCs)

PMCs are prominent class of composites compared to other composite materials in commercial applications. Polymer-matrix composites (PMCs) consist of a polymer resin as the matrix, with fibers as the reinforcement medium.

Fiber Materials: Boron, Graphite, Carbon most of the PMCs use either carbon-graphite or aramid fibers, which are the main commercial fibers

These materials are used in the greatest diversity of composite applications, as well as in the largest quantities, in light of their room-temperature properties, ease of fabrication, and cost.

In this section, the various classifications of PMCs are discussed according to reinforcement type (i.e., glass, carbon, and aramid), along with their applications and the various polymer resins that are employed.

Glass Fiber-Reinforced Polymer (GFRP) Composites
Carbon Fiber-Reinforced Polymer (CFRP) Composites
Aramid Fiber-Reinforced Polymer Composites

Glass Fiber-Reinforced Polymer (GFRP) Composites

- FRP with glass fibers are called glass fiber reinforced plastics or glass fiber reinforced polymers (GFRP).
- Glass fibers (or Fibre Glass): Easy to manufacture, chemical resistance.
- Glass fiber surface is coated with a thin polymer layer, i.e. “size” to protect the fiber surface from damage.
- GFRPs’ use temperature is limited below 200^oC due to polymer matrix.
- Major applications in automotive, marine vehicle bodies, pipes, storage containers, industrial flooring.

Carbon Fiber-Reinforced Polymer (CFRP) Composites

- FRP with carbon fibers are called carbon fiber reinforced plastics or carbon fiber reinforced polymers (CFRP).
- Matrix: Epoxy, polyester (thermosetting plastics) phenol formaldehyde.
- High specific modulus and specific strength even at high temperature.
- Good physical and mechanical properties.
- Expensive manufacturing processes.
- Major applications of CFRPs’ in aircraft structural components, sporting goods,

rocket motor cases, pressure vessels, etc.

Aramid- Fiber-Reinforced Polymer (AFRP) Composites (Kevlar)

- FRP with aramid fibers is called aramid fiber reinforced plastics or aramid fiber reinforced polymers (AFRP).
- Thermoplastic Materials: Poly-para phenylene terephthalamide (PPTP)
- High tensile properties and weak compressive properties.
- Mechanically stable between - 200 $^{\circ}$C and 200°C.
- Chemically weak to degradation by strong acids and bases.
- Major applications of AFRPs' in bullet-proof vests, sporting goods, ropes, missile cases, pressure vessels, automobile brakes.

Metal-Matrix Composites (MMCs)

- The matrix is more ductile than the reinforcements.

  The reinforcement may improve specific strength, stiffness, abrasion resistance, creep resistance, thermal conductivity, and dimensional stability of the overall composites.
- **Matrix materials**: Superalloys (eg. Single crystal Ni-based alloys), Al, Mg, Ti, Cu.
- **Reinforcements**: C, SiC, B, Al_2O_3 fibers and Al_2O_3 particles.
- **Advantages:** (i) Higher operating temperatures (ii) Non-flammability
  (iii) Greater resistance to degradation by organic fluids.
- **Disadvantages:** Expensive & higher density
- **Applications:** (i) Automobile engine components.
  (ii) Aerospace structures (eg. Space shuttle orbiter, telescope made from B or C fibers – Al matrix composites.
  (iii) Turbine engines (W fiber – superalloy composites)

3.16 Ceramic-Matrix Composites (CMCs)

- CMCs are the advanced class of structural materials consisting of metallic/non-metallic reinforcements incorporated into the ceramic matrix.
- **Matrix materials**: Silicon carbide, silicon nitride, aluminium oxide and multiple component of Al, Si & oxygen.
- **Reinforcements**: Carbon and aluminium oxide.
- **Advantages:** (i) CMCs are widely used in engineering applications where the operating temperature lies in between 800°C to 1650°C
  (ii) For use in high temperature and severe stress.
  (iii) High strength and modulus
  (iv) Very high service temperature
  (v) Reduce weight (lower fuel consumption).
- **Disadvantage:** Very brittle.
- **Applications**: (i) Automobile, aircrafts gas and turbine engines.
  (ii) Deep-see mining.
  (iii) Cutting tools and pressure vessels.

Mechanical Properties of materials

The tensile test is used to determine the mechanical properties of the materials. The following mechanical properties can be performed using tensile test.

(a) Limit of proportionality
(b) Yield point
(c) Modulus of elasticity
(d) Maximum tensile strength
(e) Breaking strength
(f) Percentage elongation
(g) Percentage reduction in area

Tensile Strength:

Tensile or Ultimate strength is the maximum load after which necking begins.

Ultimate tensile strength=Ultimate load / original cross sectional area

Creep:

Creep is a time dependent and permanent deformation of materials when subjected to constant load at a high temperature Examples:Turbine blades,Steam generators

Hardness:

Hardness is defined as the ability of a material to resist plastic deformation such as small dent in the surface, cutting, penetration and scratching.

Fatigue strength:

Definition of fatigue strength is the highest stress that a material can withstand for a given number of cycles without breaking.

Impact strength:

Impact strength is a measure of the amount of energy that a material can absorb before fracturing under a high rate of deformation.

Fracture:

Fracture can be defined as the breaking up or separation of a solid into two or more parts when subjected to an external load.

Types of Fracture:

(i) Ductile fracture

(ii) Brittle fracture

(iii) Fatigue Fracture

(iv) Creep Fracture

Ductile Fracture:

The ductile fracture is defined as the fracture which takes place by a slow propagation of crack with extensive plastic deformation.

Brittle fracture:

Brittle fracture may be defined as a fracture which takes place by a rapid propagation of crack with a negligible deformation.

Fatigue fracture:

Fatigue fracture ia defined as the fracture which takes place under repeatedly applied fatigue stresses.

Creep Fracture:

Creep fracture is the fracture that takes place due to excessive temperature of metals under steady loading.

UNIT - V

QUANTUM PHYSICS

Dual nature of radiation

In an attempt to understand the nature of light radiation, Sir Isaac Newton (1680) formulated the corpuscular theory of light. It failed to explain phenomena like interference, diffraction, and polarization. In the meantime Huygens proposed the wave theory of light, which got established as it explained most of the experimental results. In 1864, C. Maxwell proposed his electromagnetic theory in the form of four equations, called Maxwell's equations. He showed that all radiations are electromagnetic in nature and have the same speed in free space. He also proved that these radiations proceed in the form of waves with their electric and magnetic fields in planes perpendicular to each other and to the direction of propagation. The theory got established when Hertz (1887) produced electromagnetic waves in laboratory. The particle nature of radiation was again revived with the advent of Planck's quantum hypothesis which was put on a firm basis by the pioneering work of Einstein, Compton and others.

Thus, certain phenomena can only be explained by assigning a particle nature to radiation. However, the wave nature of radiation is needed to explain phenomena such as interference, diffraction, and polarization. We can therefore arrive at a conclusion that light radiation possesses a dual nature-particle and wave. At times it seems to behave like a wave and at certain other times it seems to behave like a particle. In other words, both the aspects are needed for a complete description of physical phenomena. Hence, the wave and particle aspects are complementary.

Matter wave

We noted that the classic experiments on interference, diffraction and polarization showed that the wave theory of light rests on firm experimental basis. The quantum theories developed by Planck and Einstein, and the experimental observations on photoelectric effect and Compton effect have placed the particle theory of light also on a firm basis. Hence, physicists accepted the wave-particle duality of light radiation as a reality.

de-Brogliehypothesis

In 1923, Louis de Broglie extended the concept of wave-particle duality exhibited by radiation to matter, in particular, to electrons. He was influenced by the grand symmetry of nature since the universe consists entirely of matter and radiation. He reasoned that if light can be particle like at times, and then matter can also be wave at times. Therefore, he concluded that if light has a wave-particle duality, the other component of the universe, matter, might also possess the wave-particle duality. Another reason in favor of the wave nature of matter was that it provided an explanation for the angular momentum quantization of Bohr. The wave associated with a material particle in motion is called a matter wave.

Wave packet

The wave associated with a particle in motion can only be represented by a wave disturbance that has large amplitude in the vicinity of the particle and small amplitude in regions where we do not expect to find the particle. In other words, it must be represented by a wave that is confined to a small region of space around the particle. Such a wave is called a wave packet. An ideal wave packet is represented in Fig.x. The wave packet moves with the velocity of the particle.

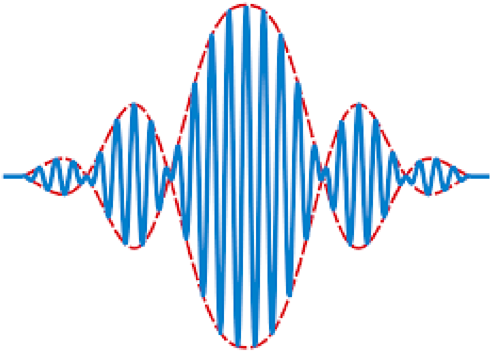


Fig. x. An ideal wave packet

de-Broglie wavelength

Photons are particles of zero rest mass. From relativity, for zero rest mass particles, we have

$$E = cp \qquad \text{(i)}$$

where$c$ is the velocity of the particle which is the velocity of light and p its momentum.

For radiation, we have

$$E = h\nu = \hbar\omega \qquad \text{(ii)}$$

Combining these two relations, we get

$$p = \frac{E}{c} = \frac{h\nu}{c} = \frac{h}{\lambda} \text{ or } \lambda = \frac{h}{p} \qquad \text{(iii)}$$

De-Broglie proposed that the wavelength and frequency of the matter wave would be related respectively to the momentum and energy by the same relationships as for a photon. Thus, for a particle of mass m and total energy$E$ travelling with speed v, the wavelength λ and frequency ν are given by,

$$\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\boldsymbol{p}} = \frac{\boldsymbol{h}}{\boldsymbol{mv}} \text{and} \nu = \frac{E}{h} \qquad \text{(iv)}$$

These are referred to as **de Broglie relations**. The wavelength λ is called the **de Broglie wavelength** of the particle.

For an electron accelerated from rest through a potential difference of V volts, assuming non-relativistic mechanics, we have

$$\frac{1}{2}mv^2 = eV \text{or} v = \sqrt{\frac{2eV}{m}} \text{(v)}$$

With this value of v, Eq. (v) reduces to

$$\lambda = \frac{h}{mv} = \frac{h}{\sqrt{2meV}} \text{(vi)}$$

Substituting the values of constants, for an electron

$$\lambda = \sqrt{\frac{150}{V} \times 10^{-10}}\, m = \sqrt{\frac{150}{V}}\, \text{Å} \qquad \text{(vii)}$$

One of the de Broglie's original arguments in favor of the wave nature of electrons was that it could give Bohr's quantization of angular momentum. Davisson and Germer (1927) and G.P. Thomson (1927) measured the wavelength of matter waves associated with the electrons in motion and confirmed de Broglie's hypothesis.

de-Broglie wavelength in terms of energy

We know that, kinetic energy (E)= $1/2mv^2$

Multiplying by 'm' on both sides we get,

$$Em = 1/2\, m^2v^2$$

Also, $m^2v^2 = 2\, Em$

$$mv = \sqrt{2Em}$$

Thus, de-Broglie wavelength, $\boldsymbol{\lambda} = \frac{\boldsymbol{h}}{\sqrt{\boldsymbol{2mE}}}$

de-Broglie wavelength in terms of voltage

When a charged particle 'e' is accelerated through a potential difference 'V'

Then the kinetic energy of the particle is given by (K.E.) = $1/2\, mv^2$ (i)

We know that energy = eV (ii)

Comparing equation (i) and (ii)

We get, $1/2\, mv^2 = eV$

Multiplying by 'm' on both sides we get

$$m^2\, v^2 = 2meV$$

Also, $mv = \sqrt{2meV}$ (iii)

Substituting equation (iii) in de-Broglie wavelength, we get

$$\lambda = \frac{h}{\sqrt{2meV}}$$

Conclusion – Properties of matter waves

- de-Broglie wavelength is inversely proportional to the velocity of the particle. If the particle moves faster, then the wavelength will be smaller and vice versa.
- If the particle is at rest, then the de Broglie wavelength is infinite. Such a wave cannot be visualized.
- de-Broglie wavelength is inversely proportional to the mass of the particle. The wavelength associated with a heavier particle is smaller than that with a lighter particle.
- de-Broglie wavelength is independent of the charge of the particle.
- Matter waves, like electromagnetic waves, can travel in vacuum and hence they are not mechanical waves.
- Matter waves are not electromagnetic waves because they are not produced by accelerated charges.
- Matter waves are probability waves, amplitude of which gives the probability of existence of the particle at the point.

The wave function

Waves on a string are described by the displacement $y\ (x,t)$ of the string. In the case of a sound wave in air, the pressure $p(x,t)$ varies in space and time. In electromagnetic waves, the fields E and B, are the ones that vary in space and time. Therefore, to characterize the de Broglie wave associated with a material particle, we require a quantity that varies in space and time. The variable quantity is called the **wave function** for the particle and is usually designated by 'Ψ' which is a function of the coordinates (x,y,z) and time t.

The displacement of a wave can either be positive or negative. In analogy, the wave function $\Psi\ (x,y,z,t)$ can have positive as well as negative values. The uncertainty principle tells us that we can only get the probability of finding the particle at (x,y,z) at time t. As probability cannot be negative, $\Psi\ (x,y,z,t)$ cannot be a direct measure of the presence of the particle. Hence, Ψ as such is not observable. But it must in some way indicate the presence of the particle, as it represents the wave associated with the particle in motion. For a particle having a well-defined momentum, the uncertainty in co-ordinate is infinite. Hence, the wave associated with it will be of infinite extent. Then, a free particle moving along x-axis with a definite momentum is described by the plane wave

$$\Psi(x,t) = Ae^{i(kx-\omega t)} \qquad \text{(i)}$$

Where $k = 2\pi/\lambda$ is the propagation constant and ω is the angular frequency.

In three dimensions, $\Psi(r,t) = Ae^{i(kr-\omega t)}$ (ii)

Such particles are non-localized particles. For a localized particle, the wave function would be represented by the wave packet.

Physical significance of wave function

Wave function is the variable quantity that is associated with a moving particle at any position (*x,y,z*) and at any time '*t*', also it relates the probability of finding the particle at that point and at that time.

- The wave function Ψ is a variable quantity.
- It is associated with a moving particle i.e., $\Psi(x, y, z, t)$ where x,y,z is the position of the particle at any time t.
- It gives information about the behaviour of the particle.
- Also it gives the statistical relation between the particle and the wave.
- $\Psi$is complex quantity and also Ψ does not have any meaning.
- But $|\Psi|^2$ has physical meaning, where$|\Psi|^2 = \Psi^* \Psi$, $\Psi^*$is the complex conjugate of Ψ.
- $|\Psi|^2$Exemplifies the probability of finding the particle per unit volume.
- $\iiint |\Psi|^2 d\tau$ represents the probability of finding the particle in a given volume $d\tau$ where $d\tau$ = dx. dy. dz
- The probability has any value between 0 and 1.
- If $\iiint \Psi^* \Psi \, d\tau = 0$ there is no particle in the given range.
- If $\iiint \Psi^* \Psi \, d\tau = 1$ there is particle certainly in the given range.
- If $\iiint \Psi^* \Psi \, d\tau = 0.5$, then, there is 50% chance for finding the particle and 50% chance for not finding the particle.
- A wave function Ψ satisfying the above relation is called a normalized wave function.

SCHRODINGER WAVE EQUATION

Classical theories of particles and waves are based on equations of motion. In quantum mechanics the state of a particle is described by the wave function Ψ (r,t). To study the motion of systems in a general way, one requires an equation of motion, which was derived by Erwin Schrodinger in 1926. This equation, called the Schrodinger equation, governs the propagation of matter waves.

Experiments have proved beyond doubt that particles exhibit wavelike properties and the wavelength of matter wave is given by the following equation as,

$$\lambda = {}^{h}/_{p} \tag{i}$$

The energy E of the particle is related to the frequency through the relation given below as follows,

$$E = h\nu = \hbar\omega \tag{ii}$$

Free Particle Wave Equation in One Dimension – Time Dependent Schrodinger Equation

A free particle moving along x-axis with a definite momentum (a non-localized particle) is described by the infinite plane wave is given by,

$$\Psi(x,\, t) = A \exp\,[i\,(kx - \omega t)] \tag{iii}$$

We know that, $k = 2\pi/\lambda = 2\pi p/h = p/\hbar$ and $\omega = E/\hbar$ (iv)

Substituting the above values in Eq. (iii), we get

$$\Psi(x,\, t) = A \exp[\tfrac{i}{\hbar}(px - Et)] \tag{v}$$

Differentiating Equation (v), with respect to x, we get

$$\frac{\partial\Psi}{\partial x} = \left(\frac{ip}{\hbar}\right) A \exp\left[\frac{i}{\hbar}(px - Et)\right] = \frac{ip}{\hbar}\Psi$$

Multiplying both sides by $-i\hbar$, we obtain

$$-i\hbar\frac{\partial\Psi}{\partial x} = p\,\Psi \tag{vi}$$

On differentiation the above equation, we get

$$\frac{\partial^2\Psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2 A \exp\left[\frac{i}{\hbar}(px - Et)\right] = -\frac{p^2}{\hbar^2}\Psi$$

Multiplying both sides by $-\frac{\hbar^2}{2m}$, we get

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = \frac{p^2}{2m}\Psi \tag{vii}$$

Differentiating Eq. (v) with respect to t gives

$$\frac{\partial\Psi}{\partial t} = \left(-\frac{iE}{\hbar}\right) A \exp\left[\frac{i}{\hbar}(px - Et)\right] = -\frac{iE}{\hbar}\Psi$$

Multiplying both sides by $i\hbar$, we get

$$i\hbar\frac{\partial\Psi}{\partial t} = E\Psi$$

(viii)

The right hand side of Equations (vii) and (viii) are equal, since for a classical particle

$$E\Psi = \frac{p^2}{2m}\Psi \qquad \text{(ix)}$$

Hence, equating the left hand sides, we get

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} \qquad \text{(x)}$$

Equation (x) is the one dimensional time dependent Schrodinger equation for a free particle.

In three dimensions, the equation becomes

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\nabla^2\Psi \qquad \text{(xi)}$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}$

Energy and Momentum Operators

Equations (viii) and (vi) can be written in the form

$\left(i\hbar\frac{\partial}{\partial t}\right)\Psi = E\Psi$ and $\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi = p\Psi$

This suggests that the energy *E* and the momentum *p* can be considered as differential operators.

Thus, we get

$$E \rightarrow i\hbar\frac{\partial}{\partial t} \text{ and } p \rightarrow -i\hbar\frac{\partial}{\partial x} \qquad \text{(xii)}$$

In three dimensions, we have

$E \rightarrow i\hbar\frac{\partial}{\partial t}$ and $p = -i\hbar\nabla$

(xiii)

General Wave Equation

The energy *E* (also called Hamiltonian) of a particle in a potential *V* is given by

$$E\Psi = \frac{p^2}{2m}\Psi + V\Psi \qquad \text{(xiv)}$$

Substituting the operators for *E* and *p*in Eq. (xiv) and allowing the resulting operator equation to operate on the wave function Ψ (*x, t*), we get

$$i\hbar\frac{\partial\Psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi\right] \qquad \text{(xv)}$$

Equation (xv) is the time-dependent Schrodinger equation for a particle moving in a potential V (x, t). The presence of i in the equation makes the solution of Ψ, in general, a complex quantity.

Schrodinger Time Independent Wave Equation

We know that time dependent wave function is given by

$$\Psi(x,\ t) = \mathrm{A}\ \exp\left[-\frac{i}{\hbar}(Et - px)\right] \qquad \text{(i)}$$

Splitting the RHS of the above equation into two parts, viz., (a) Time dependent factor and (b) Time independent factor, we can write

$$\Psi(x,\ t) = \mathrm{A}\ e^{\frac{-iEt}{\hbar}}\, e^{\frac{ipx}{\hbar}} \qquad \text{(ii)}$$

In general above equation can be written as,

$$\Psi(x,\ t) = \mathrm{A}\ \Psi e^{\frac{-iEt}{\hbar}} \qquad \text{(iii)}$$

Where the parameter Ψ represents the time independent wave function ($\Psi = e^{\frac{ipx}{\hbar}}$)

Differentiating equation (iii) partially with respect to 't', we get

$$\frac{\partial \Psi}{\partial \mathrm{t}} = \mathrm{A}\ \ \Psi\, e^{\frac{-iEt}{\hbar}}\left(\frac{-\,i\,E}{\hbar}\right) \qquad \text{(iv)}$$

Differentiating equation (iii) partially with respect to 'x', we get

$$\frac{\partial \Psi}{\partial \mathrm{x}} = \mathrm{A}\ \ e^{\frac{-iEt}{\hbar}}\frac{\partial \Psi}{\partial \mathrm{x}} \qquad \text{(v)}$$

Differentiating equation (v) again partially with respect to 'x', we get

$$\frac{\partial^2 \Psi}{\partial \mathrm{x}^2} = \mathrm{A}\ \ e^{\frac{-iEt}{\hbar}}\frac{\partial^2 \Psi}{\partial \mathrm{x}^2} \qquad \text{(vi)}$$

The Schrodinger time dependent wave equation for a free particle moving along 'x' is given by

$$i\hbar\frac{\partial \Psi}{\partial \mathrm{t}} = \left[-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial \mathrm{x}^2} + V\Psi\right]$$

(vii)

Substituting the Equation (iii), (iv) and (vi) in equation (vii), we get

$$i\hbar \mathrm{A}\ \ \Psi\, e^{\frac{-iEt}{\hbar}}\left(\frac{-\,i\,E}{\hbar}\right) = -\frac{\hbar^2}{2m}\mathrm{A}\ \ e^{\frac{-iEt}{\hbar}}\frac{\partial^2 \Psi}{\partial \mathrm{x}^2} + V\,\mathrm{A}\ \ \Psi e^{\frac{-iEt}{\hbar}}$$

(viii)

On solving,

$$i\hbar\left(\frac{-\,i\,E}{\hbar}\right)\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial \mathrm{x}^2} + V\Psi$$

$$E\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

$$E\Psi - V\Psi = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

On rewriting the above equation we get,

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \qquad \text{(ix)}$$

The above equation represents the Schrodinger time independent wave equation for a free particle moving along '*x*'.

In three dimensions, the equation becomes

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0 \qquad \text{(x)}$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Uncertainty Principle

Heisenberg, a German scientist stated the principle of uncertainty which is a consequence of dual nature of matter and waves (De Broglie Relationship). The Heisenberg uncertainty principle states that it is impossible to find the position and momentum (velocity) of an electron at the same moment. Mathematical representation of this is as follows:

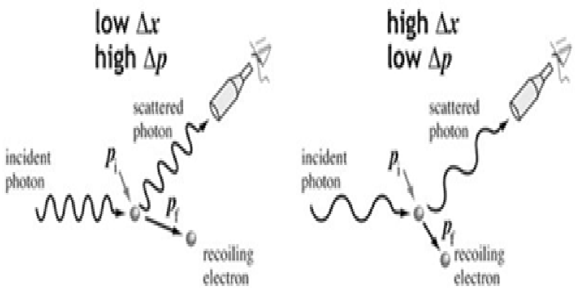
$\triangle x \times \triangle v_x \geq h/4\pi m$

$\triangle x$ is the uncertainty in position of the electron
$\triangle v_x$ is the uncertainty in the momentum (velocity)
h = Planck's Constant
m = mass

If we know the position of an electron with high accuracy then its velocity will be uncertain. Similarly, if the velocity of an electron is known precisely then its position will be uncertain. The exact picture for both, momentum and position will never be clear. This is the main concept for the principle of uncertainty.

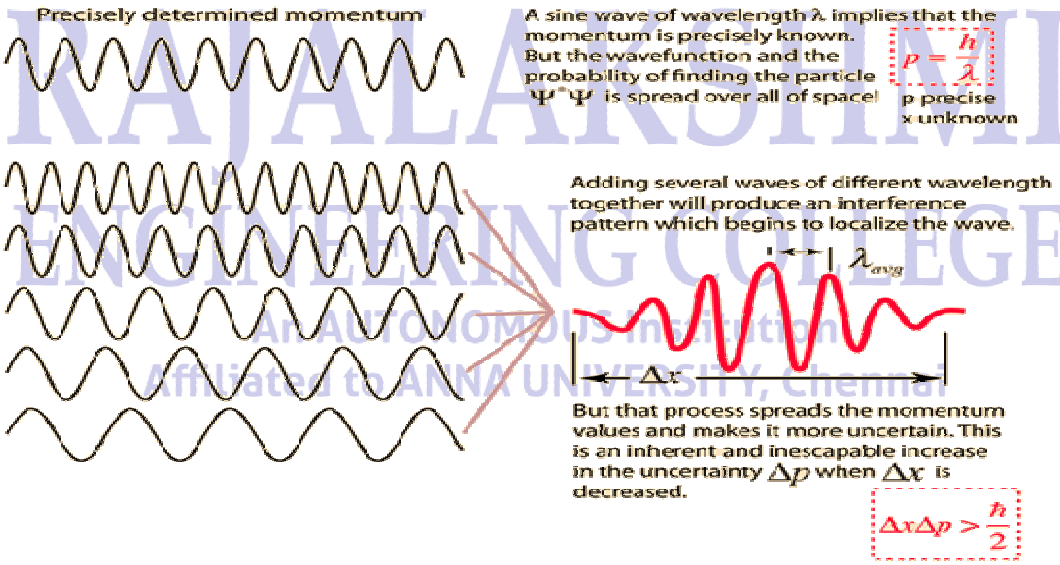
$$\Delta x \, \Delta p \geq \hbar$$

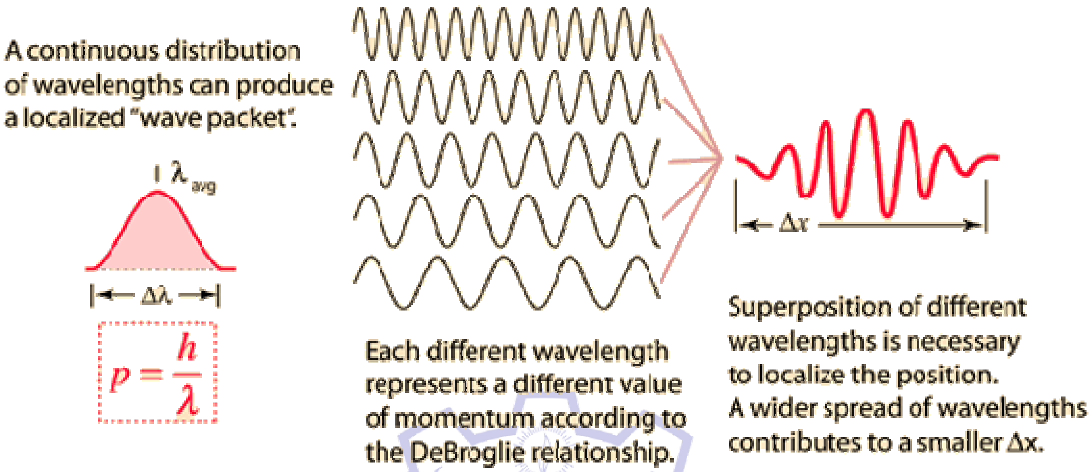
Δx = uncertainty in position
Δp = uncertainty in momentum
$\hbar$ = $h/2\pi$



Heisenberg uncertainty principle explained

Important steps on the way to understanding the uncertainty principle are wave-particle duality and the DeBroglie hypothesis. As you proceed downward in size to atomic dimensions, it is no longer valid to consider a particle like a hard sphere, because the smaller the dimension, the more wave-like it becomes. It no longer makes sense to say that you have precisely determined both the position and momentum of such a particle. When you say that the electron acts as a wave, then the wave is the quantum mechanical wavefunction and it is therefore related to the probability of finding the electron at any point in space. A perfect sinewave for the electron wave spreads that probability throughout all of space, and the "position" of the electron is completely uncertain.





Confinement Calculation

Confinement in atom

Assume atomic size = $0.4nm = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 1.66x10^{-24}\,kg \cdot m/s$$

$$\Delta p = p \;;\quad E = \frac{p^2}{2m}$$

For electron:

$$E = \frac{(1.66x10^{-24}\,kg \cdot m/s)^2}{2(9.11x10^{-31}\,kg)(1.6x10^{-19}\,J/eV)}$$

$$E = 9.4eV$$

Confinement in nucleus

Nuclear size = $\frac{1}{20,000}\,x\;0.4nm = \Delta x$

$$\Delta p = \frac{h}{\Delta x} = 3.31x10^{-20}\,kg \cdot m/s$$

For electron:

$$E = \frac{(3.31x10^{-20}\,kg \cdot m/s)^2}{2(9.11x10^{-31}\,kg)(1.6x10^{-19}\,J/eV)}$$

$$E = 3.77x10^9\,eV = 3.77GeV$$

For proton, divide by $m_p / m_e = 1836$

$$E = 2.05x10^6\,eV = 2.05MeV$$

If you examine this calculation in detail, you will note that a gross approximation was made in the relationship Δp = h/Δx. This was done to get a qualitative relationship that shows the role of Planck's constant in the relationship between Δx and Δp and thus the role of h in determining the energy of confinement. The other reason for doing it was to get an electron confinement energy close to what is observed in nature for comparison with the energy for confining an electron in the nucleus. If you actually use the limiting case allowed by the uncertainty principle, Δp = hbar/2Δx, the confinement energy you get for the electron in the atom is only 0.06 eV. This is because this approach only confines the electron in one dimension, leaving it unconfined in the other directions. For a more realistic atom you would need to confine it in the other directions as well. A better approximation can be obtained from the three-dimensional particle-in-a-box approach, but to precisely calculate the confinement energy requires the Shrodinger equation (see hydrogen atom calculation).

Particle Confinement

The uncertainty principle contains implications about the energy that would be required to contain a particle within a given volume. The energy required to contain particles comes from the fundamental forces, and in particular the electromagnetic force provides the attraction necessary to contain electrons within the atom, and the strong nuclear force provides the attraction necessary to contain particles within the nucleus. But Planck's constant, appearing in the uncertainty principle, determines the size of the confinement that can be produced by these forces. Another way of saying it is that the strengths of the nuclear and electromagnetic forces along with the constraint embodied in the value of Planck's constant determine the scales of the atom and the nucleus.

The following very approximate calculation serves to give an order of magnitude for the energies required to contain particles.

Applications of Schrodinger Wave Equation

Schrodinger wave equation has many applications. Among these, a simple problem of a particle in a potential well is discussed here.

4.11.1 Particle in a One dimensional well

Consider a particle of mass ‘m’ trapped in a one dimensional potential well of width ‘L’ as shown in fig. Since the particle is treated as a wave, the well sets the boundary conditions on the wave. According to uncertainty principle a particle confined to a finite space cannot have zero kinetic energy. Here the particle can move freely between 0 and L at constant speed and with constant kinetic energy along x direction.

The regions x<0 and x> L are forbidden. The particle cannot leave the well. The potential energy function that describes the particle in this case,

$$V(x) = \begin{cases} 0 & \text{for } 0< \; < x < \; <L \\ \infty & \text{for } x \leq 0, x \geq L \end{cases}$$

Schrodinger wave equation,

Hψ =Eψ

Where, [H=KE+PE] H is Hamiltonian operator along x- direction.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi$$

Rearranging the equation,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0 \longrightarrow (1)$$

For the region I and III, V(x) = ∞

$$\psi_I(x) = \psi_{III}(x) = 0$$

In the region II, V(x) =0

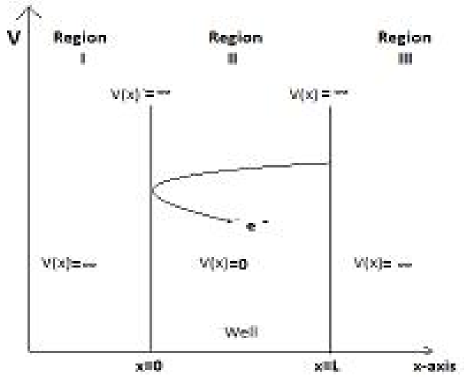


Fig. Partical in a one dimensional well

Substituting this in equation 1, we get

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \longrightarrow (2)$$

$$\frac{d^2\psi}{dx^2} + k^2 = 0 \longrightarrow (3) \quad \text{where momentum vector } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solution for this second order differential equation is,

$$\psi_{II}(x) = C\sin kx + D\cos kx \longrightarrow (4)$$

Where C and D are unknown constants to be determined. Since the particle cannot be found on the wall, and wave function is continuous, which means that $\psi(x)=0$ at both x=0 and x=L

Use boundary conditions, to find constants C and D,

If x=0, then $\psi(0)=0$

Equation (4) becomes

$$C \sin 0 + D \cos 0 = 0$$

$$D = 0$$

If x=L, then $\psi(L)=0$

$$C \sin kL = 0$$

From the above equation, either C= 0 or sinkL=0

Already D=0 if C=0 then the solution is meaningless. Hence sinkL=0

Where $kL = 0, \pm\pi, \pm2\pi, \pm3\pi \ldots. = n\pi$

Therefore $k = \frac{n\pi}{L} \longrightarrow (5)$

n=1, 2, 3….where n is any integer. Clearly n = 0 is not valid as the wavefunction vanishes.

Substituting C, D and k in equation (4) we get,

$$\psi_{II}(x) = C \sin\frac{n\pi x}{L} \longrightarrow (6)$$

Energy Eigen Value and Eigen Function

We know that, $k^2 = \frac{2mE}{\hbar^2}$

From equation (5), $k^2 = \frac{n^2\pi^2}{L^2}$

Equating these two equations, we get $E_n = \frac{n^2h^2}{8mL^2} \longrightarrow (7)$ (Generally $E = E_n$ and $\hbar = \frac{h}{2\pi}$)

Equation (7) give the value of energy of a particle inside an infinitely deep potential well. It is clear that the energy of the particle is quantized. The discrete set of allowed energies are given by,

If n=1 $E_1 = \frac{h^2}{8mL^2}$

If n=2 $E_2 = \frac{4h^2}{8mL^2} = 4E_1$

If n=3 $E_3 = \frac{9h^2}{8mL^2} = 9E_1$

If n=4 $E_4 = \frac{16h^2}{8mL^2} = 16E_1$

Where E_n be the energy Eigen value and ψ_n be the Eigen function.

Zero point energy

Even at 0k, the lowest possible energy of a particle is not zero. that is If the energy is zero , there is no kinetic energy, and the particle is stationary. Then the linear momentum becomes zero ($E = \frac{P^2}{2m}$). And for the uncertainty in the particle's position to be infinite. (the particle can never be at rest because it always has some kinetic energy. If n=0,ψ_n becomes 0) This is called the zero point energy.

The unknown constant C may be found by normalizing the wave function (the particle is physically allowed to occupy somewhere in the space) , here the particle may not be found in regions of infinite potential, so the integration limits are 0 and L.

The total probability density of finding the particle in the well is 1

Hence the square modulus of the wave function is ,

$$\int_0^L |\psi_n(x)|^2 \, dx = 1 \longrightarrow (8)$$

$$\int_0^L C^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$C^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

$$\frac{C^2}{2} \int_0^L \left[1 - \cos\left(\frac{2n\pi x}{L}\right)\right] dx = 1$$

Where $\sin^2\theta = \frac{1-\cos 2\theta}{2}$

$$\frac{C^2}{2}\left[x - \sin\frac{\left(\frac{2n\pi x}{L}\right)}{\frac{2n\pi}{L}}\right]_0^L = 1$$

$$C = \sqrt{\frac{2}{L}}$$

(9)

Substituting (9) in (6)

$$\psi_{II}(x) = \sqrt{\left(\frac{2}{L}\right)}\sin\frac{n\pi x}{L} \tag{10}$$

Equation (10) gives the wave functions of a particle trapped in an one dimensional potential well of width L.

The Discrete energy levels , their corresponding normalized wave functions and probability densities are shown in fig. (a), (b) and (c)

4.11.2 Physical interpretation of probability density function

When n = 1 the probability of finding the particle inside the well between 0 and ¼ is 0.2472 .It is maximum at x= ½ and zero at x = 0 , L. From this we can assume that at central region the probability of finding the particle is maximum and minimum at the walls.

When n = 2 the probability of finding the particle is maximum at x = L/4 and 3L/4 and zero at x = 0 ,L/2 and L ,means the particle is neither at the walls nor at the centre of the well.

When n= 3 ,ψ_3 is maximum values at x = L/6,L/2 and 5L/6 and zero at x = 0,L/3,2L/3 and L .means that the particle is neither at the walls nor at the centre of the well.

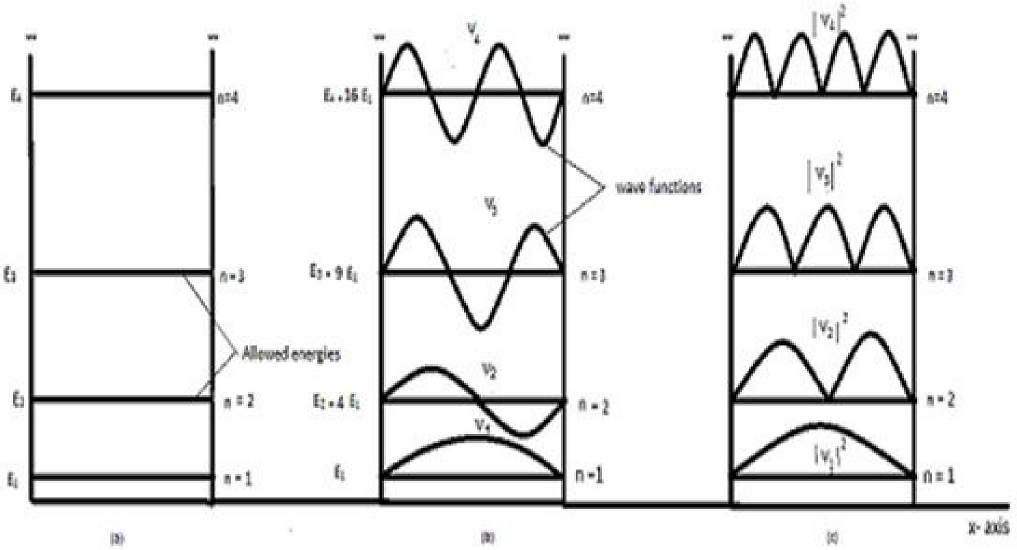


Fig. (a), (b) and (c) represents Discrete Energy levels ,wave function and probability density of a particle inside an infinite potential well

Dirac notation

By now you should be aware that QM is very mathematical. As the mathematical complexity of physics By now you should be aware that QM is very mathematical. As the mathematical complexity of physics increases, very complicated equations should be handled with very economic representations. Theoretical mathematicians in the past century have devoted great labour in the organization and abstraction of functions and algebraic structures. In doing so, physicists who were struggling with frightening equations were beginning to take advantage of what was new in math. Not surprisingly, the founders of QM did just that. To describe the physics of QM, much of the formalism is structured around functional analysis and linear operators. I will not go into too much detail on both, so I will explain why functional analysis and linear operators are so important in quantum theory.

Linear Operators in Hilbert Space

The space in which wavefunctions inhabit is determined by the four properties of wavefunctions outlined in Lecture 3. This is the Hilbert space. The Hilbert space is remarkable for many reasons, particularly in the generalization of the dot product (the inner product) in arbitrarily many dimensions (up to infinite dimensions). For technical reasons, the Hilbert space is also called the complete inner product space (here complete means linear). In QM, we need to know the following properties. I will represent everything in the Dirac notation (also known as the bra-ket notation), which is a quick and tidy way of expressing inner products.

Unit – I - Mechanics and Properties of Matter

SHORT ANSWER QUESTIONS

1. State Hooke’s law.
2. Define stress and strain. Write their units.
3. Name the types of stresses and define it.
4. Name the types of strains and define it.
5. Distinguish ductile and brittle substance.
6. Why bridges are declared unsafe after long use? Give reasons.
7. What do you infer from stress-strain diagram?
8. How does verify Hooke’s law?
9. Define hysteresis in elasticity?
10. Which is more elastic, a steel wire or rubber? Justify.
11. Define Poisson’s ratio.
12. Define lateral strain.
13. Name the three types of elastic moduli?
14. Define Young’s modulus of elasticity and mention its unit.
15. Define rigidity modulus of elasticity and mention its unit.
16. Define bulk modulus of elasticity and mention its unit.
17. Point out the factors affecting the elasticity of a material.
18. Interpret temperature affect the elasticity?
19. Interpret the addition of impurity atoms affect the elasticity of a material?
20. Interpret annealing affect the elasticity?
21. Define bending moment of a beam.
22. Define neutral axis.
23. Define uniform bending and why is it said to be uniform?
24. Distinguish uniform and non-uniform bending.
25. Point out the advantages of I shape girder?
26. Define cantilever?
27. When a wire is bent back and forth, it becomes hot. Justify?
28. Define elastic fatigue.
29. Define yield point.
30. Define moment of a force?
31. List out the uses of torsional pendulum?
32. Define angle of twist?
33. Draw stress-strain diagram for soft iron and ceramics.
34. Define torsional pendulum.
35. Define tensile strength and safety factor.

LONG ANSWER QUESTIONS

1. State and explain Hooke's law of elasticity. Draw stress-strain diagram and discuss the behavior of ductile material under loading.
2. What are the factors affecting elasticity of material and explain it.
3. Derive expression for the torsional couple per unit angular twist when a cylinder is twisted.
4. Derive an expression for the period of oscillation of a torsion pendulum. How can it be used to determine the torsional rigidity of a wire?
5. Describe the theory of torsion pendulum and explain a method to determine the moment of inertia of an irregular body.
6. Derive an expression for the internal bending moment of a beam in terms of radius of curvature.

7. What is cantilever? Obtain an expression for the depression at the loaded end of a cantilever whose other end is fixed assuming that its own weight is not effective in bending.
8. Derive an expression for depression at the free end of a cantilever due to load. Describe an experiment to determine the Young's modulus of the cantilever material using this expression.
9. A beam of length l, breadth b and thickness d is fixed at one end, the length and breadth being horizontal, and a load W is applied at the other end. If E is the Young's modulus of the material of the beam, derive an expression for the depression at the loaded end. (The weight of the beam may be assumed to be not affecting in bending).
10. Describe with necessary theory, the method to determine the Young's modulus of the material of a rectangular bar by uniform bending.
11. Explain with theory, the determination of Young's modulus of elasticity of the material of a beam, supported at its ends and loaded in the middle.
12. Discuss I shape girders.

UNIT-II - Crystal Physics
SELF EVALUATION QUESTIONS
SHORT ANSWER QUESTIONS

1. Define crystals.
2. Differentiate between crystalline and amorphous materials.
3. What is a basis?
4. Outline how a unit cell differs from a basis.
5. Describe a body centered cubic lattice.
6. Distinguish between single and polycrystalline materials.
7. Distinguish identity and inversion symmetry operations.
8. List out the seven crystal systems.
9. Illustrate the various possible lattices of an orthorhombic system.
10. Estimate the packing fraction of a simple cubic system.
11. Calculate the effective number of a BCC crystal.
12. Draw the (110) lattice plane of a cubic lattice.
13. Choose and list the primitive lattices among the Bravais lattices.
14. Sketch the unit cell of a HCP lattice.
15. Point out the significance of Miller indices.
16. Compare the coordination number of FCC and HCP lattices.
17. Define inter-planar spacing.
18. Calculate the inter-planar spacing between the (100) planes of a cubic lattice whose lattice constant is 1.056 Ȧ.
19. Write the atomic radius of a BCC lattice in terms of its lattice constant (a).
20. Justify why a lattice should be infinite.
21. Identify the material with a lower density among two crystals having FCC and SC structure.
22. What is a reciprocal lattice?
23. Write the reciprocal lattice vectors of a simple cubic lattice.
24. Why are x-rays diffracted by a crystal lattice?
25. Distinguish between interstitial and substitutional defect in a crystal.
26. Define Burger vector.
27. Illustrate a Frenkel pair.
28. What is nucleation?
29. Outline the principle of Czochralski method of crystal growth.
30. Enumerate the merits of melt growth.
31. Sketch the apparatus of Bridgmann growth technique.

LONG ANSWER QUESTIONS

1. List out, with neat sketches the 14 Bravais lattices.
2. Calculate the atomic packing fraction for SC, BCC and FCC lattices.
3. Illustrate how Miller indices of a given lattice plane can be determined.
4. Derive an expression for the inter-planar spacing in a cubic lattice in terms of the planes' Miller indices and the lattice constant.
5. Explain the concept and significance of reciprocal lattice.
6. Show that the reciprocal lattice of a FCC lattice is a BCC lattice.
7. Given that the axial ratio (c/a) of a HCP lattice is 1.6, estimate its packing fraction and show that it is equal to the packing fraction of a FCC lattice.
8. Defend that the HCP lattice is one of the two tightly packed arrangements possible while stacking a single type of atom.
9. Establish that a reciprocal lattice is the Fourier transform of a direct lattice.
10. Illustrate the various point defects possible in a crystal lattice.
11. Show how Burgers vectors are used to represent various lines defects in a crystal.
12. Explain any one of the processes of melt growth of single crystals.

Unit-III - Physics of Materials

PART A

1. **Define an alloy. (2014)**

   An ***alloy*** is a metallic, homogeneous solid mix of two or more different elements, one of which at least is essentially a metal.

   Ex. Nichrome, stainless steel, Bross, etc.,

2. **Mention the main three advantages of alloy making. (2005)**
   1. To enhance the harness of metal: Addition of 0.5 % arsenic to lead makes it so hard that it can be used for making bullets.
   2. To lowering of melting point than of its constituents elements.
   3. To enhancement of corrosion resistance than metal.

3. **What is meant by 18/8 stainless steel?**

   Austenitic Stainless steel, it contains 18% Cr and 8% Ni. It is most widely used steel and has maximum resistant to corrosion

4. **How is bronze superior to steel? (2011)**

   Bronze is a copper alloy. They posses,
   1. Low melting point than steel
   2. Better heat and electrical conductivity
   3. Greater corrosion and water resistancy than steel

5. **State the significance of increasing carbon content in steel. (2011)**

   Steel is an alloy of Iron mix with Chromium and Carbon. The content of carbon varies between 0.3-1.5% in steel. If steel contains 0.35% of carbon, it considers as non heat treatable stainless steel and it cannot with stand for higher heating. If steel contains 1.2% (increased amount) of carbon, it considers as heat treatable stainless steel and can be used up to 800^0C.

6. **What is meant by nitriding? (2011)**

   The metal alloy is heated with NH_3 at 550^0C results in super-hard surface. Nitrogen liberated from ammonia reacts with surface constituents to form extremely hard nitrides. This method is called nitriding.

7. **What are the types of phase diagrams?**

   Phase diagram is a graph obtained by plotting one degree of freedom against another. A plot of temperature (T) against pressure (P) is called P-T diagram. Similarly, a plot of temperature (T) against composition (C) is known as T-C diagram. From these diagrams, it can be understand the behaviour of system stability and equilibrium between phases.

8. **How many phases and components are present in alcohol – water system?**

   In alcohol – water system both the water and alcohol miscible completely and they will form one liquid phase with two components.

9. What is eutectic point?

Two solid substances capable of forming solid solutions having the properties of lowering each other's freezing point. The minimum freezing point corresponding to eutectic mixture is eutectic point. At eutectic point Degrees of freedom is Zero.

10. State Phase rule.

Gibbs' phase rule was proposed by Josiah Willard Gibbs in his landmark paper titled *On the Equilibrium of Heterogeneous Substances*, published from 1875 to 1878. The rule is the equality

F = P-C+2

Where *F* is the number of degrees of freedom, *C* is the number of components and *P* (alternatively π or Φ) is the number of phases in thermodynamic equilibrium with each other.

The number of degrees of freedom is the number of independent intensive variables, i. e. the largest number of properties such as temperature or pressure that can be varied simultaneously and arbitrarily without affecting one another. An example of one-component system is a system involving one pure chemical, while two-component systems, such as mixtures of water and ethanol, have two chemically independent components, and so on. Typical phases are solids, liquids and gases.

11. What is Phase diagram?

Phase diagram is a graphical representation of the physical states of a substance under different conditions of temperature and pressure. A typical phase diagram has pressure on the y-axis and temperature on the x-axis. As we cross the lines or curves on the phase diagram, a phase change occurs. In addition, two states of the substance coexist in equilibrium on the lines or curves.

12. What is triple point?

The **triple point** of a substance is the temperature and pressure at which the three phases (gas, liquid, and solid) of that substance coexist in thermodynamic equilibrium.http://en.wikipedia.org/wiki/Triple_point - cite_note-gold-1

Example: In water system all the three phases ice water and water vapour exist in equilibrium 4.58 mm of mercury and 0.0098 °C

13. What is eutectic point?

Two solid substances capable of forming solid solutions having the properties of lowering each other freezing point. The minimum freezing point corresponding to eutectic mixture is eutectic point.

14. State condensed phase rule.

If we consider the two component system of solid ↔ liquid equilibrium it is generally characterized by the absence of the vapour phase and are relatively unaffected by changes in pressure. If we keep the pressure constant of a system it will constitute a condensed system. The degree of freedom get reduced by one and for such a system the phase rule becomes

$$F' = C - P + 1$$ known as condensed (reduced) phase rule.

Two variables to be considered Viz. temp and conc. Solid-liquid equilibriums are represented on T-C diagrams.

PART B

1. State Phase rule and explain the terms involved in it.
2. Draw a neat phase diagram for one component water system.
3. Explain thermal analysis of two component alloy system.
4. Draw a neat phase diagram for Pb-Ag system and explain.
5. Draw a neat zinc-magnesium system and explain in detail. (Jan. 2014)
6. Discuss composition, properties and uses of any two non-ferrous alloys. (Jan. 2014)
7. Draw a neat two component lead-silver system and explain. (June 2014)
8. Discuss any four heat treatment of steel in detail. (June 2014)
9. Discuss the composition, properties and uses of any two ferrous alloys. (June 2014)
10. What are the uses/merits of phase diagrams?
11. Explain the composition, properties and uses of various brass.
12. Explain the composition, properties and uses of various stainless steel.

Unit-IV - Engineering Materials and Testing

PART-A

1. Define metallic glasses along with its types.

2. Define glass transition temperature.

3. Mention four applications of metallic glasses.

4. What are shape memory alloy.

5. Write a short note on Transformation temperature in SMA.

6. Differentiate martensite and Austenite.

7. Write any four applications of SMA.

8. Mention few advantages and disadvantages of SMA.

9. Define Nanotechnology & Nanomaterials?

10.What are fullerenes and clusters?

11.What are top-down and bottom-up approach?

12.Write a short note on Sol-Gel method?

13.Differentiate single wall and double wall CNT.

14.Mention some of the properties of carbon nanotubes.

15.Mention some of the properties of Nanomaterials.

16.Define ceramics.

17.What is the role of silica in clay products?

18.List some examples of white ware ceramic products.

19.What is meant by cement

20.Why are ceramics brittle in nature? Explain.

21. What are composites?

22. Define the term reinforcement and matrix.

23.What is the role of matrix?

24. What is the role of reinforcement?

25.Which type of fibre reinforced composite can be used for elevated temperature applications?

PART-B

1) Explain the characteristics, properties and applications of SMA (Shape Memory Alloy).
2) a) Write a short note on Metallic glasses.
   b) Briefly explain the melt spinning method of fabrication of metallic glasses.

c) Mention two Structural, Mechanical, Electrical & Magnetic properties of metallic glasses.

3) Briefly explain any two method of synthesis and properties of nanomatetrials.

4) Write a short on any two method of applications and properties of carbon nanotubes.

5) Describe the types, properties and applications of fibre reinforced plastics.

6) Explain the different types of ceramics in detail.

PART-A

1. **What are metallic glasses?**

   Met glasses are the amorphous metallic solids which have high strength, good magnetic properties and better corrosion resistance and wil possess both the properties of metals and glasses.
2. **What are shape memory alloys?**

   When material is heated above the transformation temp, then there will be some change in the crystal structure. Such materials are called shape memory alloys.
3. **What are nano materials? Give examples.**

   Nano materials are the materials in which the atoms size is in the order of 1 to 100 nano and these atoms will not move away from each other.

   Ex: ZnO,Ni,Pt etc.
4. **Mention properties of met glasses?**
   - ✓ Met glasses have TCP structure rather than hexagonal closely packed structure.
   - ✓ Very strong in nature.
   - ✓ They possess malleability, ductility etc.
5. **What are the properties of SMA?**
   - ✓ They have pseudo- elastic and super elastic property
   - ✓ They exhibit hysteresis curve, during cooling and beating process.
6. **Give any three applications of SMA**
   - ✓ It is used in Eye glass frames. Toys, helicopter blades.
   - ✓ They are also used in fire safety valves, coffer maker.
   - ✓ They are used in relays and activators.
7. **What are the properties of nano particles?**
   - ✓ The energy bands in these materials will be very narrow.
   - ✓ In nano materials a large number of atoms will be present at the surface.

- ✓ Interparticles spacing is very less in nano- materials.

8. List out any recent applications of nano- meterials.

- ✓ It is used in ICs,optical switches, mass sensors etc.
- ✓ Recently nano-robots were designed, which are used to remove the damaged cancer cells
- ✓ It is used in the production of DNA-chips, bio-sensors etc.

9. Define Ceramics.

Ceramics are compounds composed of both metallic and non metallic elements bonded together primarily y ionic and/or covalent bonds

10. What are composites?

Composites are combination of two materials in which one of the material is called reinforcing phase, is in the form of fibres,sheets or particles and is embedded in the other material called matrix phase.

UNIT – V - QUANTUM PHYSICS
QUESTION BANK
PART-A

1. Define blackbody and black body radiation.
2. State Wien's displacement law.
3. State Rayleigh – Jean's law.
4. State Stefan-Boltzmann's law.
5. Interpret ultraviolet catastrophe?
6. Describe the postulates of Planck's Quantum theory.
7. Write down Planck's radiation formula in terms of wavelength.
8. What is Compton Effect? (Incoherent scattering)
9. Compute Compton wavelength?
10. Calculate minimum and maximum values of Compton shift?
11. Differentiate Compton wavelength and Compton shift.
12. Photo electric and Compton effect both arise due to the action of photon on electron but the two effects are not the same. Justify.
13. Out of visible light and X-ray which can most easily show Compton effect. Support your answer?
14. State Heisenberg's uncertainty principle.
15. Describe wave function?
16. Point out some of the physical significance of the wave function.
17. Illustrate "Eigen values" and "Eigen functions"?
18. Define Photon? Give its properties.
19. Express de- Broglie wave or matter waves?
20. Explain degenerate states and non-degenerate states.
21. Express is Schrödinger wave equation?
22. Illustrate Schrödinger time independent and dependent wave equations.
23. Outline the importance of normalising a wave function?
24. Free particles in one dimensional box can have positive energy values only. Justify.
25. Write the energy value of the particle in one dimensional box.
26. Illustrate free particle? List out the parameters characterise it?
27. State the basic principle of Electron Microscope.
28. Point out any four differences between Optical and Electron microscope.
29. Illustrate any four failures of Classical Mechanics.
30. State the limitations of Optical microscope.
31. Define quantum tunnelling?
32. An X-ray photon is found to have doubled its wavelength on being scattered by 90º. Calculate the energy and wavelength of incident photon.

33. Calculate the de-Broglie wave length of an electron in the first Bohr orbit of Hydrogen atom.
34. A proton and a deuteron have the same kinetic energy. Determine the longer wavelength.
35. Calculate the uncertainty in the momentum and velocity of an electron confined in a box of length 10 nm.
36. Compute the energy of the lowest three levels for an electron in square well of width 3 Å.
37. Calculate the peak wavelength of the blackbody radiation emitted by the human body when the skin temperature is 36 ºC.

PART-B

1. Illustrate Black Body radiation .Derive the expression for Planck theory of black body radiation?
2. Define Compton Effect? Derive an expression for the Compton shift.
3. Derive an expression for de-Broglie wavelength for matter waves?
4. Illustrate de-Broglie hypothesis? Describe an experiment, which supports the existence of matter waves.
5. Derive an expression for Schrodinger time independent and dependent wave equation.
6. Explain particle in one dimensional box and also explain three dimensional effects.