**3ME4-06 : MATERIAL SCIENCE AND ENGINEERING**

**Credit: 3 Max. Marks: 150 (IA:30, ETE:120) 3L+0T+0P**

**Subject notes**

**UT-1**

Materials science is an interdisciplinary field involving the properties of matter and its applications to various areas of science and engineering. It includes elements of applied physics and chemistry, as well as chemical, mechanical, civil and electrical engineering.

**Classification of materials**

**Metals:** These materials are characterized by high thermal and electrical conductivity; strong yet deformable under applied mechanical loads; opaque to light (shiny if polished). These characteristics are due to valence electrons that are detached from atoms, and spread in an electron sea that glues the ions together, i.e. atoms are bound together by metallic bonds and weaker vander Walls forces. Pure metals are not good enough for many applications, especially structural applications. Thus metals are used in alloy form i.e. a metal mixed with another metal to improve the desired qualities. E.g.: aluminum, steel, brass, gold.

**Ceramics:** These are inorganic compounds, and usually made either of oxides, carbides, nitrides, or silicates of metals. Ceramics are typically partly crystalline and partly amorphous. Atoms (ions often) in ceramic materials behave mostly like either positive or negative ions, and are bound by very strong Coulomb forces between them. These materials are characterized by very high strength under compression, low ductility; usually insulators to heat and electricity. Examples: glass, porcelain, many minerals.

**Polymers:** Polymers in the form of thermo-plastics (nylon, polyethylene, polyvinyl chloride, rubber, etc.) consist of molecules that have covalent bonding within each molecule and van der Waals forces between them. Polymers in the form of thermo-sets (e.g., epoxy, phenolics, etc.) consist of a network of covalent bonds. They are based on H, C and other non-metallic elements. Polymers are amorphous, except for a minority of thermoplastics. Due to the kind of bonding, polymers are typically electrical and thermal insulators. However, conducting polymers can be obtained by doping, and conducting polymer-matrix composites can be obtained by the use of conducting fillers. They decompose at moderate temperatures (100 – 400 C), and are lightweight. Other properties vary greatly.

**Composite materials:** Composite materials are multiphase materials obtained by artificial combination of different materials to attain properties that the individual components cannot attain. An example is a lightweight brake disc obtained by embedding SiC particles in Al-alloy matrix. Another example is reinforced cement concrete, a structural composite obtained by combining cement (the matrix, i.e., the binder, obtained by a reaction known as hydration, between cement and water), sand (fine aggregate), gravel (coarse aggregate), and, thick steel fibers. However, there are some natural composites available in nature, for example – wood. In general, composites are classified according to their matrix materials. The main classes of composites are metal-matrix, polymer-matrix, and ceramic-matrix.

**Semiconductors:** Semiconductors are covalent in nature. Their atomic structure is characterized by the highest occupied energy band (the valence band, where the valence electrons reside energetically) full such that the energy gap between the top of the valence band and the bottom of the empty energy band (the conduction band) is small enough for some fraction of the valence electrons to be excited from the valence band to the conduction band by thermal, optical, or other forms of energy. Their electrical properties depend extremely strongly on minute proportions of contaminants. They are usually doped in order to enhance electrical conductivity. They are used in the form of single crystals without dislocations because grain boundaries and dislocations would degrade electrical behavior. They are opaque to visible light but transparent to the infrared. Examples: silicon (Si), germanium (Ge), and gallium arsenide (GaAs, a compound semiconductor).

**Biomaterials:** These are any type material that can be used for replacement of damaged or diseased human body parts. Primary requirement of these materials is that they must be biocompatible with body tissues, and must not produce toxic substances. Other important material factors are: ability to support forces; low friction, wear, density, and cost; reproducibility. Typical applications involve heart valves, hip joints, dental implants, intraocular lenses. Examples: Stainless steel, Co-28Cr-6Mo, Ti-6Al-4V, ultra high molecular weight poly-ethelene, high purity dense Al-oxide, etc.

**Crystal structures**

All metals, a major fraction of ceramics, and certain polymers acquire crystalline form when solidify, i.e. in solid state atoms self-organize to form *crystals*. Crystals possess a long-range order of atomic arrangement through repeated periodicity at regular intervals in three dimensions of space. When the solid is not crystalline, it is called amorphous. Examples of crystalline solids are metals, diamond and other precious stones, ice, graphite. Examples of amorphous solids are glass, amorphous carbon (a-C), amorphous Si, most plastics.

There is very large number of different crystal structures all having long-range atomic order; these vary from relatively simple structures for metals to exceedingly complex structures for ceramics and some polymers. To discuss crystalline structures it is useful to consider atoms as being hard spheres, with well-defined radii. In this scheme, the shortest distance between two like atoms is one diameter. In this context, use of terms *lattice* and *unit cell* will be handy. *Lattice* is used to represent a three-dimensional periodic array of points coinciding with atom positions. *Unit cell* is smallest repeatable entity that can be used to completely represent a crystal structure. Thus it can be considered that a unit cell is the building block of the crystal structure and defines the crystal structure by virtue of its geometry and the atom positions within.

Important properties of the unit cells are

• The type of atoms and their radii *R*.

• Cell dimensions (Lattice spacing a, b and c) in terms of *R* and

• Angle between the axis α, β, γ

• a\*, b\*, c\* - lattice distances in reciprocal lattice , α\*, β\*, γ\* - angle in reciprocal lattice

• *n*, number of atoms per unit cell. For an atom that is shared with *m* adjacent unit cells, we only count a fraction of the atom, 1/*m*.

• *CN*, the coordination number, which is the number of closest neighbors to which an atom is bonded.

• *APF*, the atomic packing factor, which is the fraction of the volume of the cell actually occupied by the hard spheres. *APF* = Sum of atomic volumes/Volume of cell.

Some very common crystal structures and relevant properties are listed in table

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Unit Cell**  | ***effective no. of atom*** | ***CN***  | ***a*/*R***  | ***APF***  |
| **Simple Cubic** | **1** | **6** | **4/√4** | **0.52** |
| **Body-Centered Cubic** | **2** | **8** | **4/√3** | **0.68** |
| **Face-Centered Cubic** | **4** | **12** | **4/√2** | **0.74** |
| **Hexagonal Close Packed** | **6** | **12** |  | **0.74** |

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Crystalline and Non-crystalline materials

Single Crystals: Crystals can be single crystals where the whole solid is one crystal. Then it has a regular geometric structure with flat faces.

Polycrystalline Materials: A solid can be composed of many crystalline grains, not aligned with each other. It is called polycrystalline. The grains can be more or less aligned with respect to each other. Where they meet is called a grain boundary.

Non-Crystalline Solids: In amorphous solids, there is no long-range order. But amorphous does not mean random, since the distance between atoms cannot be smaller than the size of the hard spheres. Also, in many cases there is some form of short-range order. For instance, the tetragonal order of crystalline SiO2 (quartz) is still apparent in amorphous SiO2 (silica glass).

**Miller indices:**

It is understood that properties of materials depend on their crystal structure, and many of these properties are directional in nature. For example: elastic modulus of BCC iron is greater parallel to the body diagonal than it is to the cube edge. Thus it is necessary to characterize the crystal to identify specific directions and planes. Specific methods are employed to define crystal directions and crystal planes. Methodology to define crystallographic directions in cubic crystal:

* a vector of convenient length is placed parallel to the required direction.
* the length of the vector projection on each of three axes are measured in unit cell dimensions.
* these three numbers are made to smallest integer values, known as indices, by multiplying or dividing by a common factor.
* the three indices are enclosed in square brackets, [uvw]. A family of directions is represented by <uvw>.

Methodology to define crystallographic planes in cubic crystal:

* determine the intercepts of the plane along the crystallographic axes, in terms of unit cell dimensions. If plane is passing through origin, there is a need to construct a plane parallel to original plane.
* take the reciprocals of these intercept numbers.
* clear fractions.
* reduce to set of smallest integers.
* The three indices are enclosed in parenthesis, (hkl). A family of planes is represented by {hkl}.

For example, if the x-, y-, and z- intercepts of a plane are 2, 1, and 3. The Miller indices are calculated as:

* take reciprocals: 1/2, 1/1, 1/3.
* clear fractions (multiply by 6): 3, 6, 2.
* reduce to lowest terms (already there). => Miller indices of the plane are (362).

 depicts Miller indices for number of directions and planes in a cubic crystal.



 **Imperfections in Solids**

Defects exists any all solid materials. For ease of their characterization, defects are classified on the basis of their geometry, which is realistic as defects are disrupted region in a volume of a solid. Defects are:

a. Point defects (zero-dimensional)

b. Line defects (single dimensional)

c. Surface defects (two dimensional)

d. Volume defects (three dimensional

**Point defects:**as the name implies, are imperfect point-like regions in the crystal. Typical size of a point defect is about 1-2 atomic diameters. Different point defects are explained in the following paragraphs. Figure-3.2 depicts various point defects.

A vacancy is a vacant lattice position from where the atom is missing. It is usually created when the solid is formed by cooling the liquid. There are other ways of making a vacancy, but they also occur naturally as a result of thermal excitation, and these are thermodynamically stable at temperatures greater than zero. At equilibrium, the fraction of lattice sites that are vacant at a given temperature (T) are:

 n/N=e-KT

where *n* is the number of vacant sites in *N* lattice positions, *k* is gas or Boltzmann’s constant, *T* is absolute temperature in kelvins, and *Q* is the energy required to move an atom from the interior of a crystal to its surface. It is clear from the equation that there is an exponential increase in number of vacancies with temperature. When the density of vacancies becomes relatively large, there is a possibility for them to cluster together and form voids.



An interstitial atom or interstitial is an atom that occupies a place outside the normal lattice position. It may be the same type of atom as the rest surrounding it (self interstitial) or a foreign impurity atom. Interstitial is most probable if the atomic packing factor is low.

Another way an impurity atom can be fitted into a crystal lattice is by substitution. A substitutional atom is a foreign atom occupying original lattice position by displacing the parent atom.

In the case of vacancies and foreign atoms (both interstitial and substitutional), there is a change in the coordination of atoms around the defect. This means that the forces are not balanced in the same way as for other atoms in the solid, which results in lattice distortion around the defect.

**Line defects or Dislocations:**

Line imperfections (one-dimensional defects) are also called Dislocations. They are abrupt changes in the regular ordering of atoms along a line (dislocation line) in the solid. They occur in high densities and strongly influence the mechanical properties of material. They are characterized by the Burgers vector (**b**), whose direction and magnitude can be determined by constructing a loop around the disrupted region and noticing the extra inter-atomic spacing needed to close the loop. The Burgers vector in metals points in a close packed lattice direction. It is unique to a dislocation.

Dislocations occur when an extra incomplete plane is inserted. The dislocation line is at the end of the plane. Dislocations can be best understood by referring to two limiting cases - Edge dislocation and Screw dislocation.

**Edge dislocation** is characterized by a Burger’s vector that is perpendicular to the dislocation line. It may be described as an edge of an extra plane of atoms within a crystal structure. Thus regions of compression and tension are associated with an edge dislocation. Because of extra incomplete plane of atoms, the atoms above the dislocation line are squeezed together and are in state of compression whereas atoms below are pulled apart and experience tensile stresses. Edge dislocation is considered positive when compressive stresses present 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 ┬. A schematic view of edge dislocations



**Figure-3.3:** *Edge dislocations.*

A pure edge dislocation can glide or slip in a direction perpendicular to its length i.e. along its Burger’s vector in the slip plane (made of ***b*** and ***t*** vectors), on which dislocation moves by slip while conserving number of atoms in the incomplete plane. It may move vertically by a process known as climb, if diffusion of atoms or vacancies can take place at appropriate rate. Atoms are added to the incomplete plane for negative climb i.e. the incomplete plane increases in extent downwards, and vice versa. Thus climb motion is considered as non-conservative, the movement by climb is controlled by diffusion process.

Screw dislocation or Burgers dislocation has its dislocation line parallel to the Burger’s vector. 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”. A schematic view of a negative screw dislocation.

 

**Fifure-3.4:** *Negative* s*crew dislocation*.

A screw dislocation does not have a preferred slip plane, as an edge dislocation has, and thus the motion of a screw dislocation is less restricted than the motion of an Edge dislocation. As there is no preferred slip plane, screw dislocation can cross-slip on to another plane, and can continue its glide under favorable stress conditions. However, screw dislocation can not move by climb process, whereas edge dislocations can not cross-slip.

Dislocations more commonly originate during plastic deformation, during solidification, and as a consequence of thermal stresses that result from rapid cooling. Edge dislocation arises when there is a slight mismatch in the orientation of adjacent parts of the growing crystal. A screw dislocation allows easy crystal growth because additional atoms can be added to the ‘step’ of the screw. Thus the term screw is apt, because the step swings around the axis as growth proceeds. Unlike point defects, these are not thermodynamically stable. They can be removed by heating to high temperatures where they cancel each other or move out through the crystal to its surface. Virtually all crystalline materials contain some dislocations. The density of dislocations in a crystal is measures by counting the number of points at which they intersect a random cross-section of the crystal. These points, called etch-pits, can be seen under microscope. In an annealed crystal, the dislocation density is the range of 108-1010 m-2.

**Volume defects**

**Interfacial defects** can be defined as boundaries that have two dimensional imperfections in crystalline solids, and have different crystal structures and/or crystallographic orientations on either side of them. They refer to the regions of distortions that lie about a surface having thickness of a few atomic diameters. For example: external surfaces, grain boundaries, twin boundaries, stacking faults, and phase boundaries. These imperfections are not thermodynamically stable, rather they are meta-stable imperfections. They arise from the clustering of line defects into a plane.

**External surface**: The environment of an atom at a surface differs from that of an atom in the bulk; especially the number of neighbors (coordination) at surface is less. Thus the unsaturated bonds of surface atoms give rise to a surface energy. This result in relaxation (the lattice spacing is decreased) or reconstruction (the crystal structure changes). To reduce the energy, materials tend to minimize, if possible, the total surface area.

**Grain boundaries:** Crystalline solids are, usually, made of number of grains separated by grain boundaries. Grain boundaries are several atoms distances wide, and there is mismatch of orientation of grains on either side of the boundary as shown in figure-3.6. When this misalignment is slight, on the order of few degrees (< 10°), it is called low angle grain boundary. These boundaries can be described in terms of aligned dislocation arrays. If the low grain boundary is formed by edge dislocations, it is called tilt boundary, and twist boundary if formed of screw dislocations. Both tilt and twist boundaries are planar surface imperfections in contrast to high angle grain boundaries. For high angle grain boundaries, degree of disorientation is of large range (> 15°). Grain boundaries are chemically more reactive because of grain boundary energy. In spite of disordered orientation of atoms at grain boundaries, polycrystalline solids are still very strong as cohesive forces present within and across the boundary.

 

 **Figure-3.6:** *Schematic presentation of grain boundaries*

**Twin boundaries:** It is a special type of grain boundary across which there is specific mirror lattice symmetry. Twin boundaries occur in pairs such that the orientation change introduced by one boundary is restored by the other (figure-3.7). The region between the pair of boundaries is called the twinned region. Twins which forms during the process of recrystallization are called annealing twins, whereas deformation twins form during plastic deformation. Twinning occurs on a definite crystallographic plane and in a specific direction, both of which depend on the crystal structure. Annealing twins are typically found in metals that have FCC crystal structure (and low stacking fault energy), while mechanical/deformation twins are observed in BCC and HCP metals. Annealing twins are usually broader and with straighter sides than mechanical twins. Twins do not extend beyond a grain boundary.

 

 **Figure-3.7:** *A pair of twin boundaries.*

**Stacking faults:** They are faults in stacking sequence of atom planes. Stacking sequence in an FCC crystal is ABC ABC ABC …, and the sequence for HCP crystals is AB AB AB…. When there is disturbance in the stacking sequence, formation of stacking faults takes place. Two kinds of stacking faults in FCC crystals are: (a) ABC AC ABC…where CA CA represent thin HCP region which is nothing but stacking fault in FCC, (b) ABC ACB CABC is called *extrinsic* or *twin stacking fault*. Three layers ACB constitute the twin. Thus stacking faults in FCC crystal can also be considered as submicroscopic twins. This is why no microscopic twins appear in FCC crystals as formation of stacking faults is energetically favorable. Stacking fault energy varies in range 0.01-0.1 J/m2. Lower the stacking fault energy, wider the stacking fault, metal strain hardens rapidly and twin easily. Otherwise, metals of high stacking fault energy i.e. narrower stacking faults show a deformation structure of banded, linear arrays of dislocations.

Phase boundaries exist in multiphase materials across which there is sudden change in physical/chemical characteristics.

**Bulk or Volume defects**

Volume defects as name suggests are defects in 3-dimensions. These include pores, cracks, foreign inclusions and other phases. These defects are normally introduced during processing and fabrication steps. All these defects are capable of acting as stress raisers, and thus deleterious to parent metal’s mechanical behavior. However, in some cases foreign particles are added purposefully to strengthen the parent material. The procedure is called dispersion hardening where foreign particles act as obstacles to movement of dislocations, which facilitates plastic deformation. The second-phase particles act in two distinct ways – particles are either may be cut by the dislocations or the particles resist cutting and dislocations are forced to bypass them. Strengthening due to ordered particles is responsible for the good high-temperature strength on many super-alloys. However, pores are detrimental because they reduce effective load bearing area and act as stress concentration sites.

**Deformation of metals**

When a sufficient load is applied to a metal or other structural material, it will cause the material to change shape. This change in shape is called deformation. A temporary shape change that is self-reversing after the force is removed, so that the object returns to its original shape, is called elastic deformation. In other words, elastic deformation is a change in shape of a material at low stress that is recoverable after the stress is removed. This type of deformation involves stretching of the bonds, but the atoms do not slip past each other**.**



**Elastic deformation**

Elastic deformation is reversible i.e. recoverable. Up to a certain limit of the applied stress, strain experienced by the material will be the kind of recoverable i.e. elastic in nature. This elastic strain is proportional to the stress applied. The proportional relation between the stress and the elastic strain is given by Hooke’s law, which can be written as follows:

 σ∝ε

 σ=Eε

where the constant E is the modulus of elasticity or Young’s modulus,

Though Hooke’s law is applicable to most of the engineering materials up to their elastic limit, defined by the critical value of stress beyond which plastic deformation occurs, some materials won’t obey the law. E.g.: Rubber, it has nonlinear stress-strain relationship and still satisfies the definition of an elastic material. For materials without linear elastic portion, either tangent modulus or secant modulus is used in design calculations. The tangent modulus is taken as the slope of stress-strain curve at some specified level, while secant module represents the slope of secant drawn from the origin to some given point of the σ-ε curve,

 

**Figure-4.1:** *Tangent and Secant moduli for non-linear stress-strain relation.*

If one dimension of the material changed, other dimensions of the material need to be changed to keep the volume constant. This lateral/transverse strain is related to the applied longitudinal strain by empirical means, and the ratio of transverse strain to longitudinal strain is known as *Poisson’s ratio* (*ν*). Transverse strain can be expected to be opposite in nature to longitudinal strain, and both longitudinal and transverse strains are linear strains. For most metals the values of *ν* are close to 0.33, for polymers it is between 0.4 – 0.5, and for ionic solids it is around 0.2.

Stresses applied on a material can be of two kinds – normal stresses, and shear stresses. Normal stresses cause linear strains, while the shear stresses cause shear strains. If the material is subjected to torsion, it results in torsional strain. Different stresses and corresponding strains are shown in figure-4.2. 

**Plastic deformation**

When the stress applied on a material exceeds its elastic limit, it imparts permanent non-recoverable deformation called plastic deformation in the material. Microscopically it can be said of plastic deformation involves breaking of original atomic bonds, movement of atoms and the restoration of bonds i.e. plastic deformation is based on irreversible displacements of atoms through substantial distances from their equilibrium positions. The mechanism of this deformation is different for crystalline and amorphous materials. For crystalline materials, deformation is accomplished by means of a process called slip that involves motion of dislocations. In amorphous materials, plastic deformation takes

place by viscous flow mechanism in which atoms/ions slide past one another under applied stress without any directionality.

Plastic deformation is, as elastic deformation, also characterized by defining the relation between stresses and the corresponding strains. However, the relation isn’t simpler as in case of elastic deformation, and in fact it is much more complex. It is because plastic deformation is accomplished by substantial movement of atomic planes, dislocations which may encounter various obstacles. This movement becomes more complex as number slip systems may get activated during the deformation.

The analysis of plastic deformation, and the large plastic strains involved is important in many manufacturing processes, especially forming processes. It is very difficult to describe the behavior of metals under complex conditions. Therefore, certain simplifying assumptions are usually necessary to obtain an amenable mathematical solution. Important assumptions, thus, involved in theory of plasticity are neglecting the following aspects:

(i) Anelastic strain, which is time dependent recoverable strain.

(ii) Hysteresis behavior resulting from loading and un-loading of material.

(iii) Bauschinger effect – dependence of yield stress on loading path and direction.

The relations describing the state of stress and strain are called *constitutive equations* because they depend on the material behavior. These relations are applicable to any material whether it is elastic, plastic or elastic-plastic. Hooke’s law which states that strain is proportional to applied stress is applicable in elastic range where deformation is considered to be uniform. However, plastic deformation is indeed uniform *but* only up to some extent of strain value, where after plastic deformation is concentrated the phenomenon called *necking*. The change over from uniform plastic deformation to non-uniform plastic deformation is characterized by ultimate tensile strength (*σu*). As a result of complex mechanism involved in plastic deformation and its non-uniform distribution before material fractures, many functional relations have been proposed to quantify the stress-strain relations in plastic range.

|  |  |
| --- | --- |
| Elastic deformation  | Plastic deformation  |
| Reversible  | Not reversible  |
| Depends on initial and final states of  | Depends on loading path  |
| stress and strain  |  |
|  |  |
| Stress is proportional to strain  | No simple relation between stress and strain  |
| No strain hardening effects  | Strain hardening effects  |

A true stress-strain relation plotted as a curve is known as *flow curve* because it gives the stress (*σ*) required to cause the material to flow plastically to any given extent of strain (*ε*) under a se

**Mechanisms of plastic deformation in metals**

Plastic deformation, as explained in earlier section, involves motion of dislocations. There are two prominent mechanisms of plastic deformation, namely **slip** and **twinning**.

Slip is the prominent mechanism of plastic deformation in metals. It involves sliding of blocks of crystal over one other along definite crystallographic planes, called slip planes. In physical words it is analogous to a deck of cards when it is pushed from one end. Slip occurs when shear stress applied exceeds a critical value. During slip each atom usually moves same integral number of atomic distances along the slip plane producing a step, but the orientation of the crystal remains the same. Steps observable under microscope as straight lines are called slip lines.

Slip occurs most readily in specific directions (slip directions) on certain crystallographic planes. This is due to limitations imposed by the fact that single crystal remains homogeneous after deformation. Generally slip plane is the plane of greatest atomic density, and the slip direction is the close packed direction within the slip plane. It turns out that the planes of the highest atomic density are the most widely spaced planes, while

the close packed directions have the smallest translation distance. Feasible combination of a slip plane together with a slip direction is considered as a slip system. The common slip systems are given in *table-6.1*.

Table-6.1: Slip systems for different crystal structures.

|  |  |  |  |
| --- | --- | --- | --- |
| **Crystal** | **Occurrence** | **Slip planes** | **Slip directions** |
| FCC |  |  {111} |  <110> |
| BCC | More common Less common | {110} {112},{123} |  <111> |
| HCP | More common Less common | Basal plane Prismatic & Pyramidal planes | Close packed directions |
| NaCl |  | {110} | <110> |

In a single crystal, plastic deformation is accomplished by the process called slip, and sometimes by twinning. The extent of slip depends on many factors including external load and the corresponding value of shear stress produced by it, the geometry of crystal structure, and the orientation of active slip planes with the direction of shearing stresses generated. Schmid first recognized that single crystals at different orientations but of same material require different stresses to produce slip. The dependence of various factors has been summarized using a parameter – critical resolved shear stress, *τR*, given as

 $τ\_{r}$=$\frac{PCOSλ}{A/COS∅}$=$\frac{P}{A}$cos$∅$cos$λ$= $σ$cos$∅$cos$λ$

m= cos$∅$cos$λ$

where *P* – external load applied, *A* – cross-sectional area over which the load applied, *λ* – angle between slip direction and tensile axis, *ø* – angle between normal to the slip plane and the tensile axis and *m* – Schmid factor.

Shear stress is maximum for the condition where *λ* = ø = 45 ْ. If either of the angles are equal to 90 ْ, resolved shear stress will be zero, and thus no slip occurs. If the conditions are such that either of the angles is close to 90 ْ, crystal will tend to fracture rather than slip. Single crystal metals and alloys are used mainly for research purpose and only in a few cases of engineering applications.

Almost all engineering alloys are polycrystalline. Gross plastic deformation of a polycrystalline specimen corresponds to the comparable distortion of the individual grains by means of slip. Although some grains may be oriented favorably for slip, yielding cannot occur unless the unfavorably oriented neighboring grains can also slip. Thus in a polycrystalline aggregate, individual grains provide a mutual geometrical constraint on one other, and this precludes plastic deformation at low applied stresses. That is to initiate plastic deformation, polycrystalline metals require higher stresses than for equivalent single crystals, where stress depends on orientation of the crystal. Much of this increase is attributed to geometrical reasons.



**Recovery, Recrystallization and Grain Growth**

As mentioned in earlier sections, annealing is an important industrial process to relieve the stresses from cold working. During cold working grain shape changes, while material strain hardens because of increase in dislocation density. Between 1-10% of the energy of plastic deformation is stored in material in the form of strain energy associated with point defects and dislocations. On annealing i.e. on heating the deformed material to higher temperatures and holding, material tends to lose the extra strain energy and revert to the original condition before deformation by the processes of recovery and recrystallization. Grain growth may follow these in some instances.

 **Recovery**

This is the first stage of restoration after cold working where physical properties of the cold-worked material are restored without any observable change in microstructure. The properties that are mostly affected by recovery ate those sensitive to point defects, for example – thermal and electrical conductivities. During recovery, which takes place at low temperatures of annealing, some of the stored internal energy is relieved by virtue of dislocation motion as a result of enhanced atomic diffusion. There is some reduction, though not substantial, in dislocation density as well apart from formation of dislocation configurations with low strain energies. Excess point defects that are created during deformation are annihilated either by absorption at grain boundaries or dislocation climbing process. Stored energy of cold work is the driving force for recovery.

 **Recrystallization**

This stage of annealing follows after recovery stage. Here also driving force is stored energy of cold work. Even after complete recovery, the grains are still in relatively high strain energy state. This stage, thus, involves replacement of cold-worked structure by a new set of strain-free, approximately equi-axed grains i.e. it is the process of nucleation and growth of new, strain-free crystals to replace all the deformed crystals. It starts on heating to temperatures in the range of 0.3-0.5 Tm, which is above the recovery stage. There is no crystal structure change during recrystallization. This process is characterized by recrystallization temperature which is defined as the temperature at which 50% of material recrystallizes in one hour time. The recrystallization temperature is strongly dependent on the purity of a material. Pure materials may recrystallizes around 0.3 Tm, while impure materials may recrystallizes around 0.5-0.7 Tm.

There are many variables that influence recrystallization behavior, namely amount of prior deformation, temperature, time, initial grain size, composition and amount of recovery prior to the start of the recrystallization. This dependence leads to following empirical laws:

- A minimum amount of deformation is needed to cause recrystallization.

- Smaller the degree of deformation, higher will be the recrystallization temperature.

- The finer is the initial grain size; lower will be the recrystallization temperature.

- The larger the initial grain size, the greater degree of deformation is required to produce an equivalent recrystallization temperature.

- Greater the degree of deformation and lower the annealing temperature, the smaller will be the recrystallized grain size.

- The higher is the temperature of cold working, the less is the strain energy stored and thus recrystallization temperature is correspondingly higher.

- The recrystallization rate increases exponentially with temperature.

During recrystallization, the mechanical properties that were changes during deformation are restored to their pre-cold-work values. Thus material becomes softer, weaker and ductile. During this stage of annealing impurity atoms tend to segregate at grain boundaries, and retard their motion and obstruct the processes of nucleation and growth. This solute drag effect can be used to retain cold worked strength at higher service temperatures. Presence of second phase particles causes slowing down of recrystallization – pinning action of the particles.

 **Grain growth**

This stage follows complete crystallization if the material is left at elevated temperatures. However, grain growth does not need to be preceded by recovery and recrystallization; it may occur in all polycrystalline materials. During this stage newly formed strain-free grains tend to grow in size. This grain growth occurs by the migration of grain boundaries. Driving force for this process is reduction in grain boundary energy i.e. decreasing in free energy of the material. As the grains grow larger, the curvature of the boundaries becomes less. This results in a tendency for larger grains to grow at the expense of smaller grains. In practical applications, grain growth is not desirable. Incorporation of impurity atoms and insoluble second phase particles are effective in retarding grain growth.

Because the driving force for grain growth is lower than the driving force for recrystallization, grain growth occurs slowly at a temperature where recrystallization occurs at substantially high speeds. However, grain growth is strongly temperature dependent.