BASIC PRINCIPLES OF PHYSICAL METALLURGY I

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INTRODUCTION

Performance of metals and alloys in actual service is primarily determined by the nature and distribution of microconstituents present. These can be seen under microscope using suitable metallographic techniques which will be discussed in detail in subsequent lectures. However, in order to interpret them it is necessary to have some elementary knowledge about the evolution of structure in metals and alloys as they solidify from melt and how this can be altered by various thermal and mechanical processes to suit specific applications. Metals and alloys have certain unique properties which are characteristic of their bonding and crystal structures. As a consequence a wide range of microstructures having different properties could be developed even in the same metal or alloy. The subject of physical metallurgy primarily deals with these. In this lecture I shall try to present some of the basic concepts of this subject so that it helps you understand and interpret the information hidden within the microstructure.

CRYSTALLINE NATURE OF METALS

Fig.1 gives a typical microstructure of a pure metal. This consists of several grains separated by distinct boundaries. Each grain represents a crystal having an orientation distinctly different from its neighbours. Often this is evident from the varying lustre of the grains. A perfectly random orientation will ensure that the metal is isotropic. In certain alloys these may be preferentially arranged (e.g. directionally solidified alloy) to exploit specific properties of crystal orientation. The size of the grains in commercial alloys can also be widely varied. Imagine that the blades of a modern aero gas turbine is made of a single grain of Ni base super alloy.

The atoms in a crystal are arranged in a periodic fashion. This is often represented by an array of regularly arranged points in space called lattice where each point has identical surroundings. Structures of most of the common metals can be represented by following three crystal structures.

(i)   FCC (face centered cubic) - Cu, Ni,. Ag, Au, Al, γ Fe

(ii)   BCC (Body centered cubic) - α Fe, Mo, W, Cr, β Ti

(iii)   Hexagonal closed packed (HCP) - Zn, Cd, Mg, Zn, αTi

Fig.2 represents the arrangement of atoms in the above crystal structures. In terms of point lattice the first two correspond to BCC & FCC lattice with one atom per lattice point, where as HCP structure is represented by hexagonal lattice with two atoms/lattice point. Incidentally there is a close similarity of atomic packing between FCC and HCP structure. The planar arrangement of atoms in the most close packed plane of both of these are identical. The only difference lies in the relative sequence in which these planes are arranged. Assuming atoms to be similar to hard ping pong balls it can be shown there are three distinct positions a close packed plane of atoms can occupy. viz. A, B, C (see Fig.2). In HCP the sequence in which these are arranged is ABABAB... where as in FCC it is ABCABC. In comparison to these two the packing density of BCC structure is a little lower. This is why when iron is cooled from γ Fe stage to α Fe there is an increase in volume of about 5%.

The close packed planes are also the furthest apart. This makes metal amenable to large plastic deformation. This takes place through glide (or slip) of a part of the crystal over the other. There is no change in relative crystal orientation on either side of the glide plane. If you deform (slightly) a piece of polished metal (for metallographic examination) and examine under microscope you would notice slip steps in various grains. They point along specific crystallographic directions. However, if you repolish and examine, the steps would vanish. This is because glide does not change orientation of one part of the crystal with respect to the other (Fig.3).

The ease with which a metal can deform depends on the availability of sufficient number of slip systems which denotes a specific combination of glide plane and glide direction. FCC crystals have the optimum number of slip system (12) where as HCP has only three slip systems of which only two are independent. This make HCP metal more difficult to deform. In crystals leaving limited slip system plastic deformation is facilitated by another mode of deformation called twinning. Here a part of the crystal rotates to take up a position which corresponds to a mirror image of the other. Therefore there is a distinct change in orientation. Deformation twins are therefore visible even after the deformed metal is repolished (Fig.3).

BCC crystals on the other hand has a large number of slip systems(48). This is because the packing density of three the sets of crystal planes are quite close. As a result slip on one system is hindered by those on the others. This also promotes formation of deformation twins. In addition the slip bands in BCC metal tend to be wavy. Nevertheless because of the availability of sufficient number of slip systems and deformation modes metal crystals can be moulded into any arbitrary shapes by plastic deformation. Examination of microstructure can clearly reveal the operative slip system and deformation modes.

PLASTIC DEFORMATION

Theoretical strength of metallic crystal is unusually high (G/10). Although most metals deform easily at a stress as low as G/10,000.

This is because all crystals have defects called dislocations. This is a line on the slip plane separating slipped and yet to slip region. Around the dislocations the atoms are displaced from their normal positions (Fig.4). This indicates that the defects have their own stress field and stored strain energy. In many instances one part of the crystal around a dislocation has a tensile stress field where as the other a compressive stress field. Such dislocations can move very easily with applications of a very low stress as the net work done is very small.

Dislocations can be seen under transmission electron microscope. The points of intersection of dislocation with the plane of the microstructure can also be seen under an optical microscope using special etching technique. Deformation of metal or slip is directly related to the movement of dislocation. Indeed often the density of dislocation is taken as the measure of plastic deformation a metal has undergone. Fig.5 shows a typical stress-strain diagram of a single crystal. Its nature is a strong function of its orientation.

If the tensile axis of the crystal lies along an axis of high symmetry (e.g cube axis) then slip occurs through movement of dislocations simultaneously on several slip systems. Many of these may intersect each other generating dislocation locks which prevents further movements., as a result there is significant strain hardening. Whereas axis having minimum symmetry initially exhibits large deformation with little strain hardening, subsequently with further deformation the axis rotates to take up a symmetric orientation when this too exhibits strain hardening. To deform them further applied stress must be raised. Finally a stage is reached when the stress is high enough for the dislocation to overcome obstacles through cross slip. As a result strain hardening rate decreases.

Stress-strain response of a polycrystalline metal is likely to be similar to that of a crystal having a high symmetry tensile axis. Here all crystals irrespective of their orientation are subjected to same arbitrary strain. This is possible only if slip takes place simultaneously on at least 5 independent slip system because 3D strain has six components and volume strain is zero. With deformation the shape of the grains changes. They get elongated along the direction of tensile axis. Microstructural examination clearly reveals such changes. Slip being a simple shear has a component of rotation as well. Therefore with deformation orientation of grains also keeps on changing. In case of very large plastic deformation majority of the grains tend to have similar crystal axes aligned along the tensile direction. The metal thus develops a characteristic deformation texture. Examination under optical microscope cannot detect such tenures. Textured metals and alloys alter the intensity ratio of various X-ray diffraction lines. Texture can also be detected by TEM. Since crystals have different properties along different directions (anisotropy), a highly deformed metal which in a way resembles single crystal is also likely to exhibit similar behaviour. This behaviour of metals and alloys is being commercially exploited as well. High tensile strength of cold drawn wires is partly due to its specific texture.

HEAT TREATMENT OF DEFORMED METAL

A deformed metal has high elastic stored energy because of increased dislocation density (10^{10} to $10^{12}/cm^2$). Therefore thermodynamically it is unstable and it has a sufficient driving force for microstructural rearrangement so as to bring down the magnitude of stored energy. This however cannot happen without thermal activation. When this is heated the dislocations attain additional mobility through the movement of vacancies by diffusion. As a result they arrange themselves in positions of minimum energy. A few of the dislocations can get annihilated as well. Deformed metals have dislocations of opposite nature separated by obstacles. When vacancy diffusion helps them overcome the barrier they come closer and ultimately get annihilated. Such rearrangement of dislocation structure within a deformed metal is known as recovery. As a result internal stresses are relieved though there is little drop in hardness (Fig.6) Rearrangement of dislocations leads to the formation of (dislocation) small angle boundary which is often visible under optical microscope. However, the shapes of all deformed grains remain unchanged.

Further heating promotes recrystallization when the deformed grains are replaced by new strain free crystals having minimum dislocation density. The process takes place through nucleation and growth. The nucleus of a strain free grain has a critical size which depends on the magnitude of cold work. Fig.6 shows that higher the cold work smaller is the critical nucleus and lower is the thermal activation required for recrystallization. Heavily cold worked metal on heat treatment (called annealing) therefore gives fine grain structure. As a result of recrystallization there is a sharp drop in hardness.

The new grains depending on the nature and distribution of second phase particles (if any) or the extent of prior cold work may or may not have random orientation. Cold worked aluminium killed steel develops a special texture due to the pressure of AlN. This is particularly suitable for deep drawing which requires high degree of planer isotropy but very a high resistance to deformation along the direction of the thickness.

Continued annealing leads to grain growth and further loss of hardness. Fig.7 shows the sequence of microstructural change during annealing of cold worked metal. FCC metals do not form deformation twin. However, some of these on annealing after cold work exhibit recrystallized grains with annealing twins. Microstructures of annealed Cu, Brass and austenitic steel often show such twins. Their presence indicates they must have been cold worked before annealing.

At this stage it is necessary to have an idea of the temperature at which recrystallization takes place. Although the exact temperature may depend on the amount of working, most metals recrystallize at Tm/3 where Tm represents the melting point in degree absolute. Therefore (plastic) deformation of low melting metal such as lead, zinc etc. at room temperature would be accompanied with recrystallization. Indeed this would technically correspond to hot working.

ALLOY

An alloy is a mixture of several elements. The earliest synthetic alloy men learned to use were brass and bronze. The former is a mixture of copper and zinc whereas the latter is a mixture of copper and tin. Steel which is the most widely used material of construction today is primarily an alloy of Fe and carbon. Most metals in their liquid state are soluble in all proportions. However as they solidify often there is a segregation. The solidified alloy consist of a number of different phases each having a separate crystalline identity. This depends on the ability of metals to accommodate atoms of other elements within its lattice. There are two distinct ways this can happen. If the second atom is very small in comparison to the parent metal it could go into the interstitial space. However, the extent to which this is possible is very limited. Therefore there is a solubility limit. Atoms like C and N form such solutions with Fe. It is interesting to compare the solubility limits of such elements in the two crystalline forms of Fe namely ferrite (α) and austenite(γ). The former being BCC is less closely packed than the latter which is FCC yet the solubility of carbon in γ is around 2.0 wt % in comparison to that of about 0.02 wt % in α. This is because BCC structure has more number of such sites than FCC lattice. In addition this is not symmetric which results in lattice distortion. This marked difference in the solubility of carbon in the two forms of iron lattice makes steel amenable to a number of heat treatments resulting in widely different microstructures. This will be dealt with in subsequent lectures.

Alternatively the atom of the second element could replace some of the atoms of the parent metal in the lattice. The capacity to do so would depend on the dimensions of the two atoms, their valencies and crystal structure. In case the size difference is within 15%, the valencies and the crystal structures are identical, the capacity to replace the parent atom could be unlimited. Under such circumstances, the two elements (metals) are miscible in all proportion in solid state. Some of the examples of such alloys are Cu Ni, CuAu. In most other cases there is a definite solubility limit. As these alloys solidify there may be phase separation. The number of phases will depend on the number of constituents. In case of binary alloys the maximum number of phases are two where as for ternary alloys it is three. The temperature range over which such phase separation takes place as the alloy solidifies are represented in the form of a phase diagram.

PHASE DIAGRAM

A pure metal is expected to solidify at a fixed temperature. However, to form nuclei of solid in a molten metal some amount of supercooling is necessary. This provides the energy required to create a new solid liquid interface which was so far nonexistent. However as a few stable nuclei form the temperature of the metal rises again to its melting point and remains constant until the process of solidification is complete. The magnitude of supercooling determines the size and the number of nuclei that form in a liquid metal. High supercooling

promotes formation of a large number of very fine nuclei whereas low supercooling gives only few large nuclei. The structure of the solidified metal can thus be controlled.

When a molten metal is allowed to solidify in a mould, a large number of stable nuclei develop along the mould wall. As the heat is extracted through the mould wall a few of them having a preferred orientation grow inwards. Finally as the temperature of the core goes below the melting point a large number of nuclei form which could grow in all possible directions. Thus three distinct zones of microstructure develops. The chilled layer is located close to the mould wall. This is followed by rather coarse columnar grains exhibiting the direction of heat flow and then the equiaxed zone near the core. Many applications may demand an uniform fine grained structure. For this the casting must be hot forged. Structure of the casting could also be refined by inoculation where certain chemicals are injected into the melt. This provides additional interfaces within the melt to facilitate nucleation.

An alloy on the other hand would solidify over a range of temperature. Let us consider the case of unlimited solubility in the solid state. Fig.8 represents the typical cooling curves of metal A&B the two constituents of the alloy. Melting point of A is greater than that of B. An alloy belonging to the system would solidify over a range of temperature which may lie between Ta and Tb. A typical cooling curve for such an alloy has also been shown in Fig.8. The temperature range over which the transformation takes place would depend on the composition. A phase diagram (Fig.8) is a graphical representation of the temperature range over which the process of solidification takes place. The line representing the temperature at which the first nucleus of solid solution forms is called the liquidus whereas the line representing the temperature at which the last trace of liquid disappears is called the solidus. In between the two temperatures both solid and liquid phase coexist. The composition of the two can be determined from the intersection of the horizontal tie line drawn at the specific temperature.

Let us examine how the phase diagram helps us understand the evolution of microstructure in an alloy belonging to this system. As the temperature goes just below the liquidus a few crystals of solid solution α forms. Its composition is given by the solidus at that temperature. Solidification proceeds as the temperature decreases with precipitation of more α having different compositions. The process continues until all the liquid is replaced by solid. It should be noted that as the solidification continues the composition of solid already precipitated out must also change.

However, the movement of atoms in solid being much slower than that in liquid this does not take place. Therefore, the composition of grains in the solidified alloy is not uniform. The central region is rich in A (the parent metal) whereas the grain boundary is rich in B (the solute). This phenomenon is known as coring. In addition, solidified casting here exhibit irregular shaped long crystals

called dendrites in place of columnar grains found in pure metals (Fig.9). Cast structure can be refined by prolong homogenization heat treatment at high temperature and hot working.

The phase diagram thus provides a basic idea about how the transformations take place in an alloy as it solidifies. Most commercial alloys have more than one alloying element, Some of these might be present as impurities which would segregate towards the grain boundary making it stronger than the matrix This is why most cast alloys exhibit better high temperature properties. Segregation is also responsible for embrittlement. Indeed embrittled microstructure gives rise to intergranular fracture. Therefore while examining a failed component the microstructure of the grain boundary regime is so carefully examined. Modern microanalytical tool can also give as an idea of the elements segregated along the grain boundary.
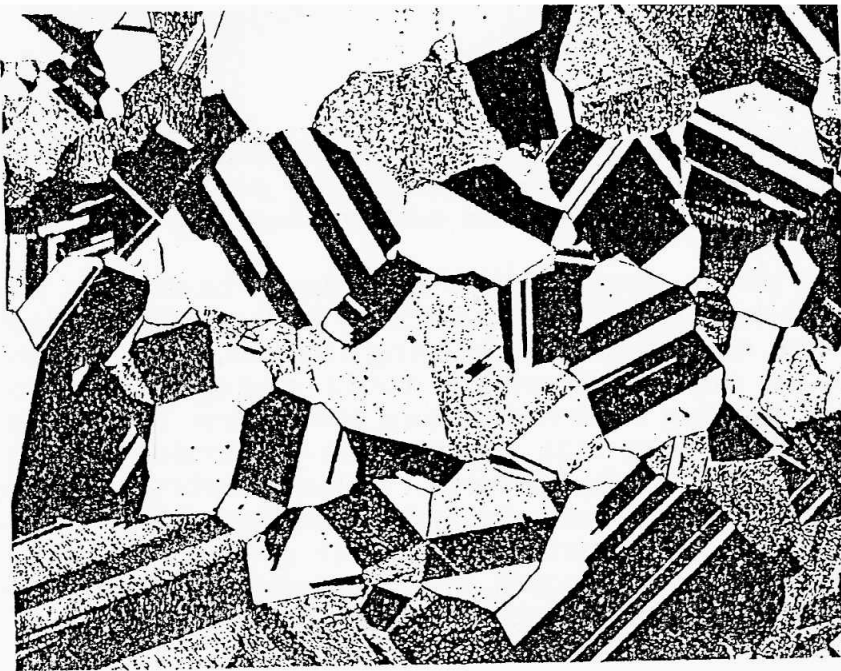
Fig.1 : A typical microstructure of a pure metal/a single phase alloy

HCP   FCC

Unit cells

BCC
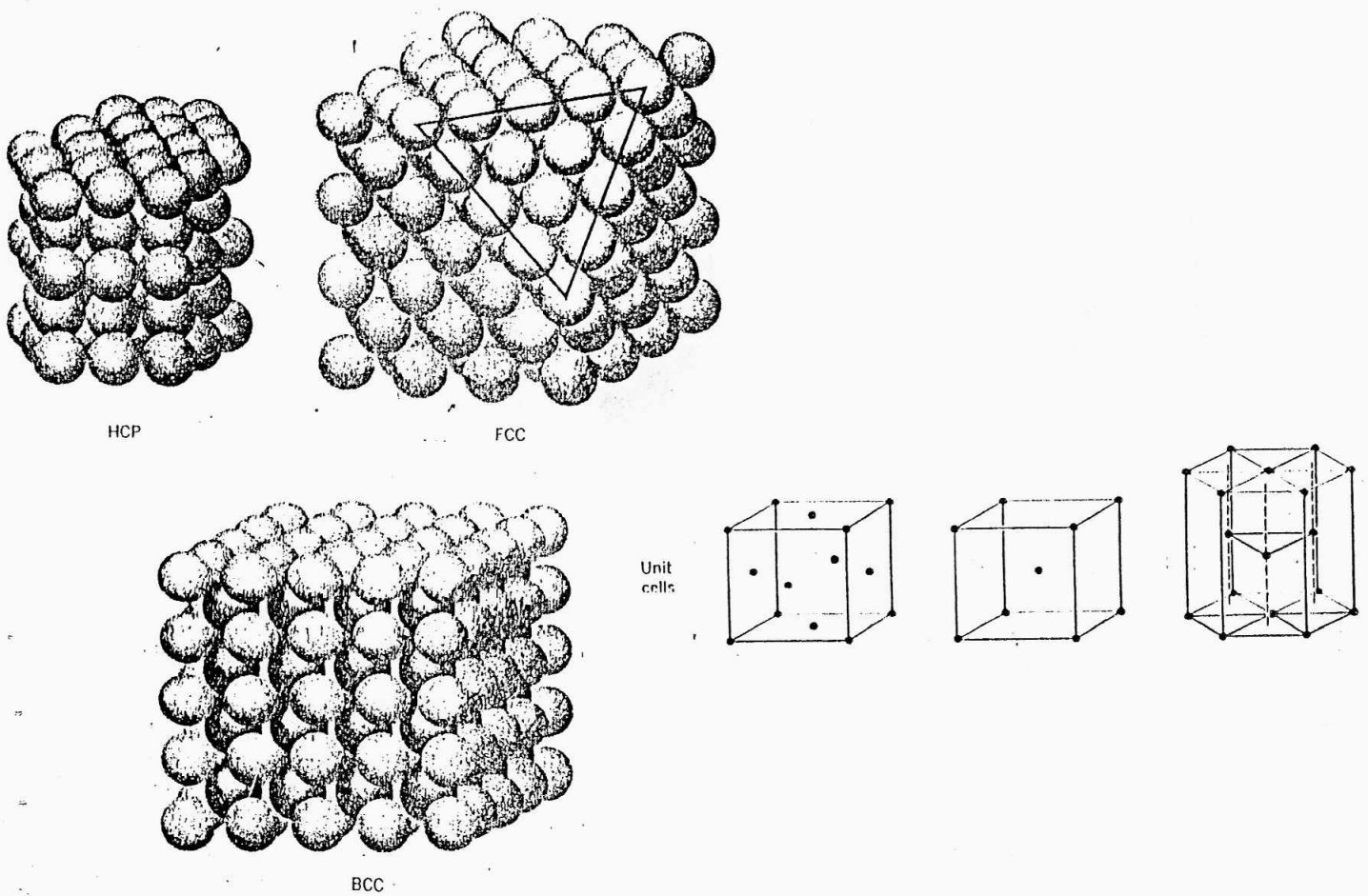
Fig.2 : Arrangements of atoms in HCP, FCC and BCC crystals
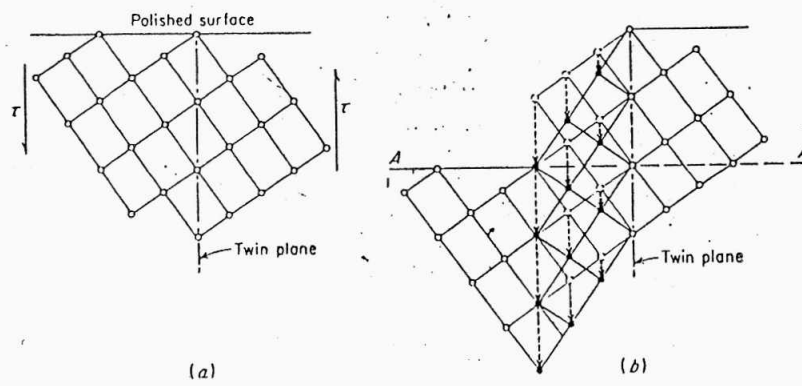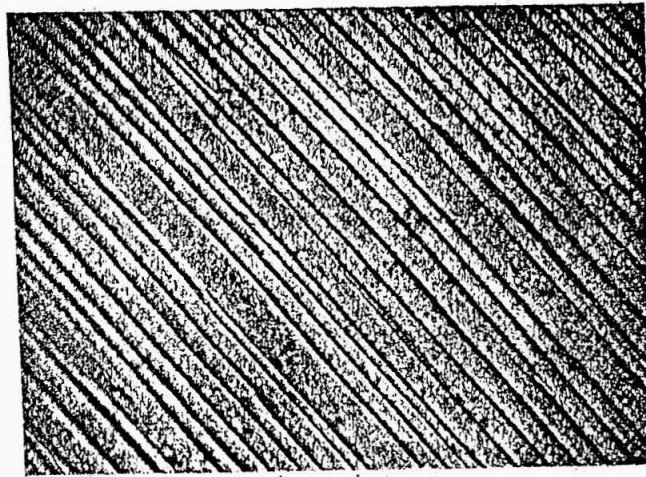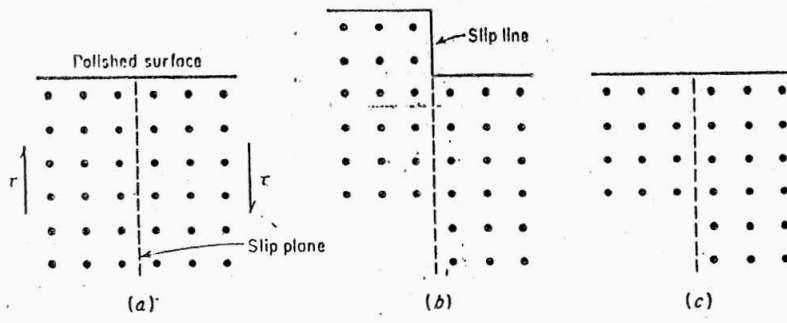
Fig.3 : Atomic movements during slip and twinning
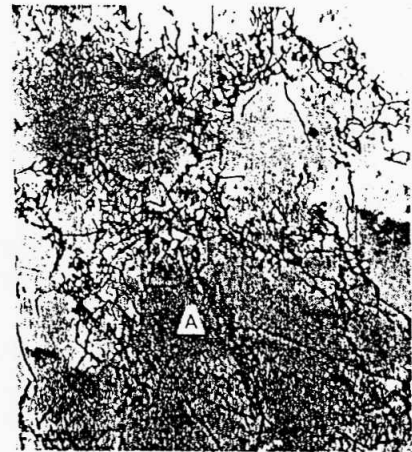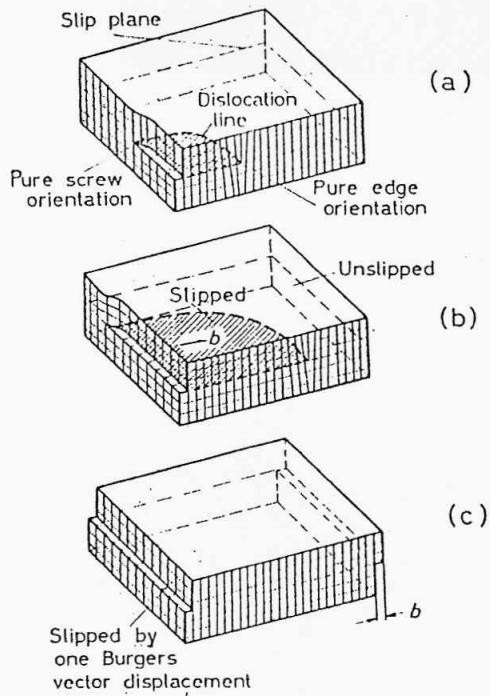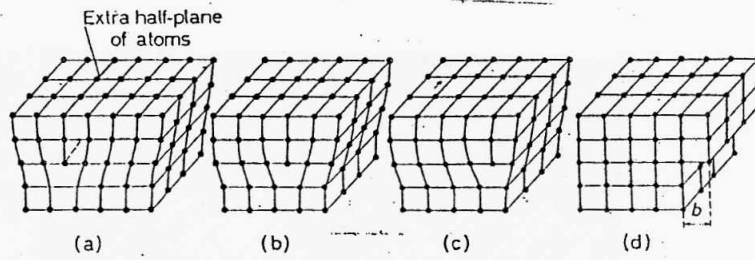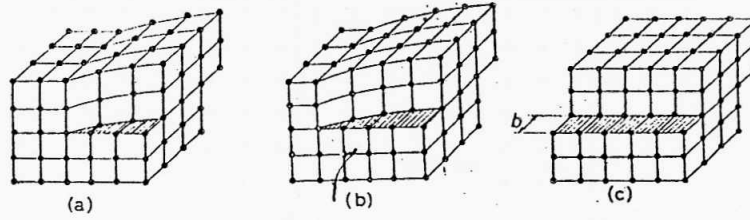
Fig.4 : Atomic arrangements around a dislocation and the
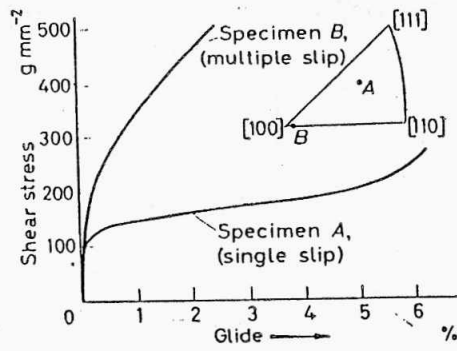process of deformation through slip
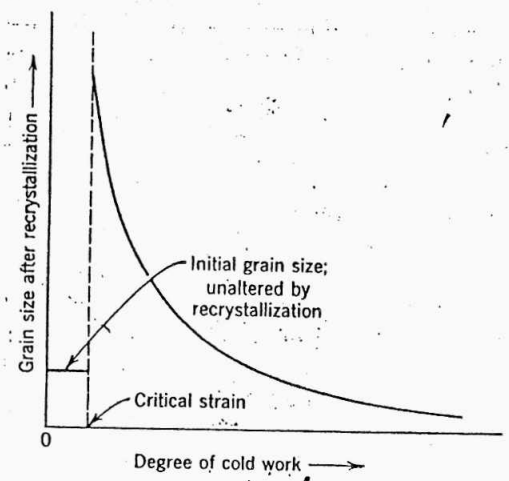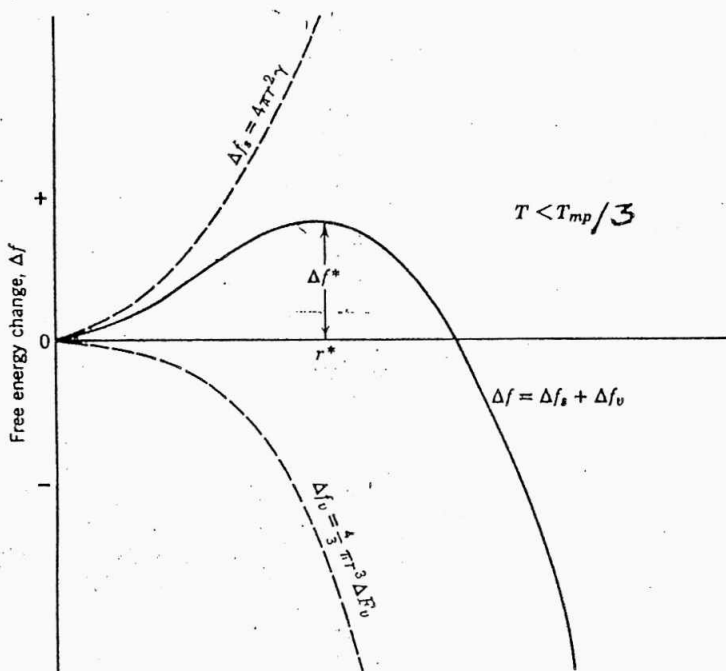
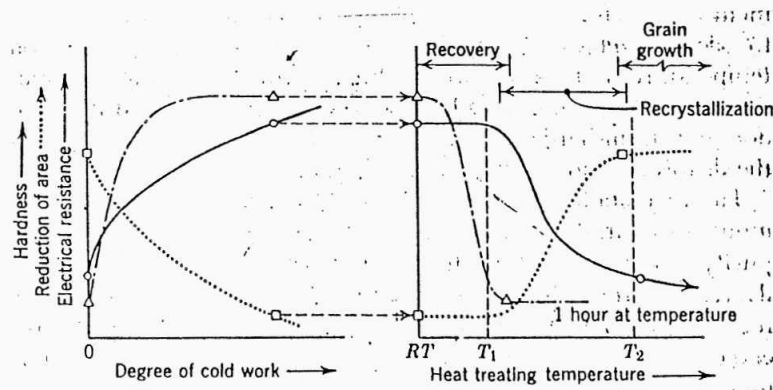Fig.5 : Typical stress-strain diagram of a single crystal
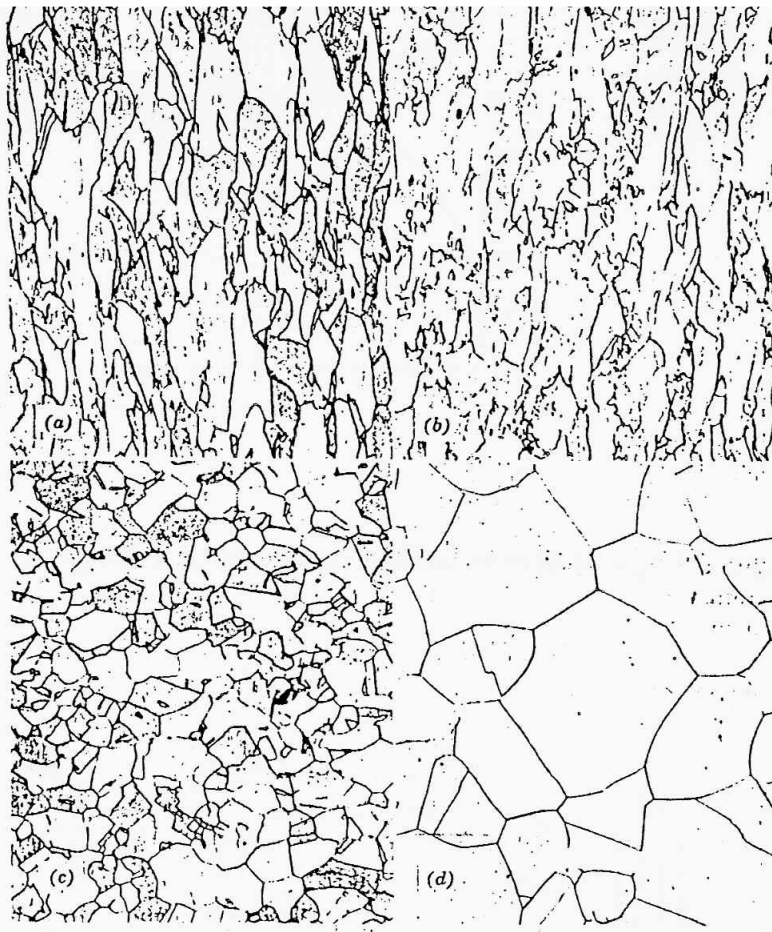

Fig.6 : Kinetics of recrystallization

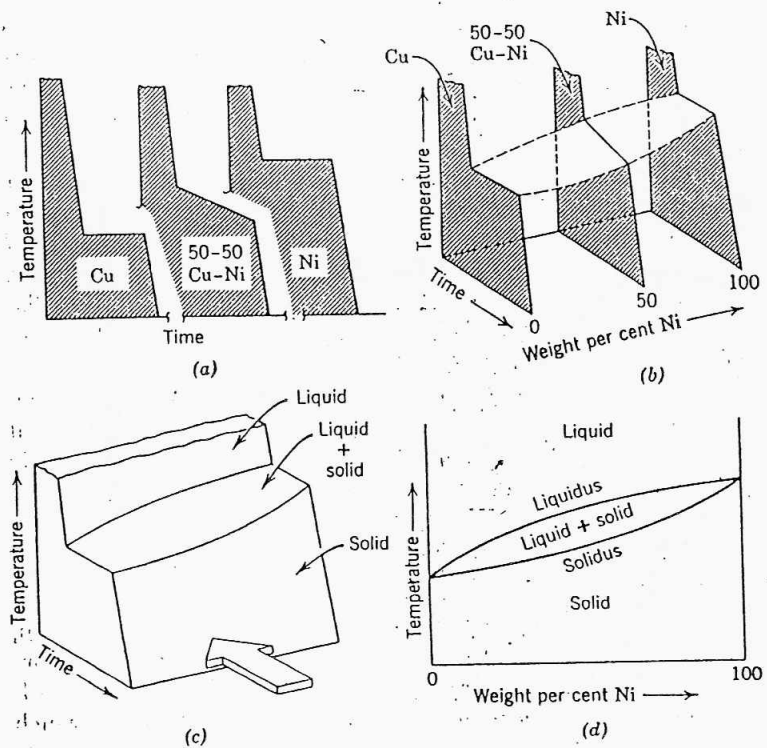Fig.7 : Sequence of microstructural change during annealing of cold worked metal

Fig.8 : Cooling curves of pure metal and binary alloys exhibiting unlimited solubility and corresponding phase diagram
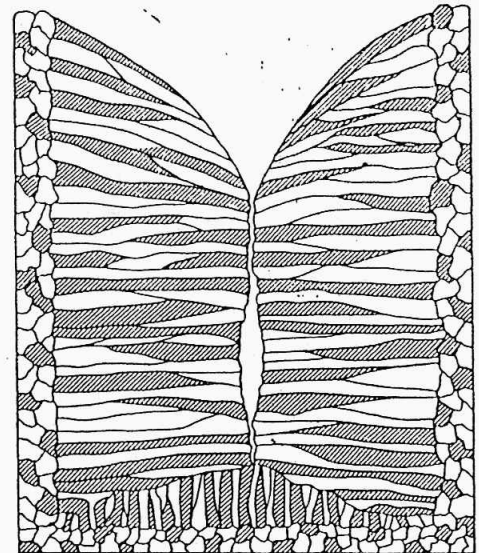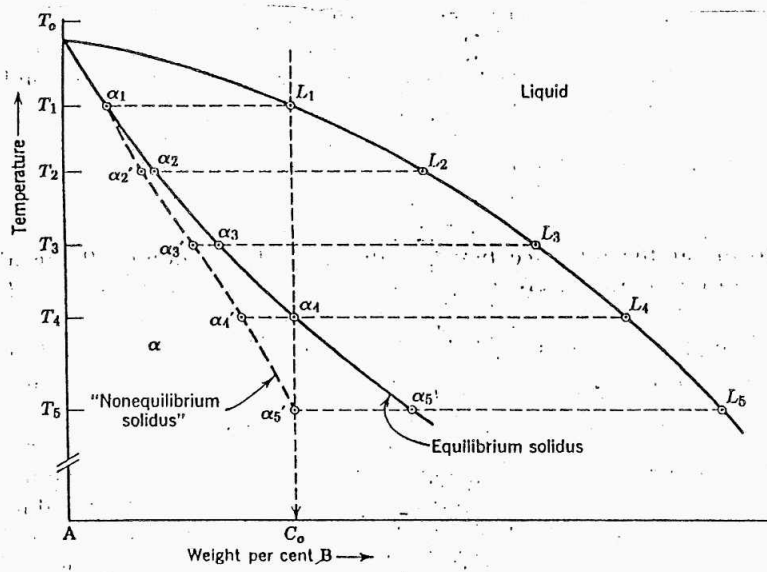
Fig.9 : (a) Effect of non-equilibrium cooling
(b) Dendritic and columnar structure