CRYSTAL STRUCTURE

We know that when most materials change their state from liquid to solid their atomic particles (atoms, ions or molecules) form into regular repeating patterns.

The particles occupy positions in what we call a "space lattice" to form crystalline substances.

Most of the chemical elements are metals and they are by far the most important materials in manufacturing. The majority of our work in Materials Science will be concerned with metals and their structure, their behaviour under load and temperature change and their properties.

Such properties as strength, conductivity, ability to be deformed without fracture and relatively high density make them ideal for use both as items of manufacture and as tools and machinery used in manufacturing.

SPACE LATTICE

The space lattice concept is used to describe the crystalline structure of materials.

We imagine that the space occupied by an amount of material is divided into equal volumes by a network of lines. This network is, of course, three dimensional.

It has been shown that only 14 different lattices are possible.

The structure for the majority of the useful metals fall into one or other of the three lattices described in Topic 2 (Bonding).

We will restrict our investigations of crystal structure to these three. They are:

2. Face-centred Cubic (F.C.C.).
3. Hexagonal close Packing (H.C.P.).

1. THE BODY-CENTRED CUBIC LATTICE

Iron (at room temperature), chromium, tungsten and molybdenum are the main metal examples of this lattice structure.

This is NOT an example of close packing of atoms.

In this lattice the lines of the network are arranged so that each line is equi-distant from its neighbours thus producing a series of cubes in space. (Figure 1).
Showing atom centres in a B.C.C. lattice. Atoms in layers A and B are indicated.

Fig. 1.

The distance between the lines is 1.155 times the atomic diameter "d". Figure 2 shows a layer of atoms placed so that the atom centres are at the intersection of the lines at the bottom level (A) in Figure 1.

Fig. 2.

Figure 3 shows a similar layer of atoms (layer B) arranged so that they occupy the valleys between the atoms of layer A.

Fig. 3.

If a third layer is arranged so that its atoms are immediately above those of layer A, effectively we have another layer A and we say the stacking is A B A B A B ....
This is an example of B.C.C structure. The atoms are in contact only along the diagonals of the cubes and so each has only 8 nearest or contact neighbours.

The number 8 is called the co-ordination number of this particular lattice structure.

Figure 4 shows a body-centred cubic unit cell.

2. THE FACE-CENTRED CUBIC LATTICE

Aluminium, copper, lead and nickel are examples of this structure. (Iron also appears as F.C.C. at temperatures between 910°C and 1400°C).

This is an example of close packing.

In this lattice the lines are equi-distant from their neighbours and so it is cubic but their spacing is equal to the atomic diameter "d".

Figure 5 shows layer A with the atoms arranged so that each is in contact with six others.

Hexagonal and triangular units are shown shaded.

This is the closest the atoms can be packed.

Figure 6 reproduces the hexagonal unit from layer A and shows the six valleys alternately shaded and clear.
The layer placed above the hexagonal unit (layer A) can only contain three atoms. This is the triangular unit from Figure 5 and let us assume these atoms occupy the shaded valleys. This becomes layer B.

There are two options for placing the next layer (layer C). If the atoms are positioned above the clear valleys in Figure 6 we have a Face-centred Cubic structure (F.C.C.).

The fourth layer will form so that each of its atoms will be immediately above those in layer A.

We say that the stacking for F.C.C. structure is ABCABCB.....

In this packing each atom has 12 nearest or contact neighbours and so this lattice structure has a co-ordination number of 12.

Figure 7 shows an F.C.C. unit cell.

3. THE HEXAGONAL CLOSE PACKING LATTICE

Zinc, Cadmium, Magnesium, Cobalt and Titanium are examples of this structure.

As with F.C.C., H.C.P. is an example of close packing.

In this lattice the spaces between the lines in two directions are equal to "d" but the distance between lines in the third direction is always greater than "d".
The first two layers A and B are laid down in the same way as in F.C.C. For the third layer however, the atoms are placed immediately above those in layer A (See Figure 8).

![Layer A](image)

**Fig. 8.**

The stacking for H.C.P. is ABAB.....

As with F.C.C. each atom will have 12 nearest or contact neighbours and so this lattice structure also has a co-ordination number of 12. Figure 9 shows an H.C.P. unit cell.

![Layer A](image)

**Fig. 9.**

**DEFORMATION**

One of the most important tasks carried out in engineering is the use of force to change the shape of materials.

Operations such as forging, rolling, drawing, extrusion and spinning are examples of how the engineer uses controlled forces to change the shape of metals.
If a piece of metal is acted on by a force, some measure of deformation will occur. The magnitude of the force will not only determine the degree of deformation but also whether the deformation is temporary or permanent.

**ELASTIC DEFORMATION:** This is the first stage of deformation and is reversed when the force is removed.

i.e. The material returns to its original shape.

The distortion produced during this stage is proportional to the magnitude of the applied force. If we double the force we double the strain. (Hooke's Law).

**Figure 10** shows diagrammatically:

(a) An unstressed unit crystal.
(b) A crystal strained by a tensile force.
(c) A crystal strained by a compressive force.

Fig. 10.

**Figure 11** shows elastic strain in a crystal structure. The strain is elastic as long as the atoms don't move away from their original neighbours.

Fig. 11.

**PLASTIC DEFORMATION:** The second stage is plastic deformation and this is not reversible. When the force is removed most of the deformation remains.

The distortion produced during this stage is not proportional to the applied force.
Figure 12 shows the stress/strain (force/deformation) diagram for a typical metal.

It can be seen that in the plastic stage relatively small increases in stress produce large increases in strain.

![Stress vs Strain Diagram]

**Fig. 12.**

We have seen from the work done in Topic 2 (bonding) that the atoms of metals (crystalline structures) are held together in a lattice form by bonding forces.

In the elastic stage the applied forces are not sufficient to overcome the atomic bonding forces. When the force is removed the bonding forces reform the atoms into their original structure.

In the plastic stage however, the applied forces are sufficient to break the atomic bonding forces and layers of atoms slide over one another to take up new positions in the lattice structure.

This process of layers of atoms sliding over one another is called "slip".

Figure 13 shows diagramatically the two stages of deformation.
**SLIP:** Figure 14 illustrates the mechanism of slip resulting in permanent deformation.

Figure 14 (a) shows two layers of atoms unstressed. When a stress load is applied the atoms of one layer "climb" out of their valleys and sit on top of their adjacent atoms. Figure 14 (b) shows this.

Figure 14 (c) shows the layer now displaced a distance equal to one atomic diameter and the atoms of this layer are now occupying the valleys adjacent to their original positions.

This is oversimplified and is provided only as a general idea of how slip occurs.

In fact the process of slippage is a progressive one where a few atoms only of adjacent layers distort and recover. This distortion and recovery proceeds along the layer until the complete layer has been displaced.

Figure 15 (a) shows the metal unstressed.

Figure 15 (b) and (c) show the few distorted atoms as they progress from left to right.

Figure 15 (d) shows the layer displacement completed.
SLIP PLANES: Microscopic examination of a material under stress shows that slip does not occur indiscriminately.

It occurs along a particular plane or layer and continues until interrupted by an irregularity or obstruction in that plane.

Slip will then begin on a different plane and so on until all available planes have been used.

At this stage any increase in stress will cause the crystal structure to remain distorted.

Slip has the effect of relieving internal stresses set up by the deforming force. If the applied force is not sufficient to cause slip the internal stresses build up and the material will become hard and brittle.

A material possessing high levels of unrelieved internal stress is said to be work hardened.

Increases in the applied force which cause slip to continue will result in failure.

Of all the forces which can cause deformation, three are relevant at this stage. They are:
Most metals will fail in shear before they will fail in either tension or compression.

i.e. Failure takes place by slippage before atomic bonding forces are completely overcome.

We have seen that slippage occurs by progressive layers or planes of atoms sliding over one another.

To do this atoms must "climb" out of their respective valleys and "drop" into adjacent ones. (See Figure 14).

It is clear that the directions in which the planes of atoms move will be the ones which require the least force to "lift" the individual atoms out of their valleys so that they may "drop" into the next valley.

These will be the directions in which the atoms are the most dense.

In Figure 16, the three distances marked "x", "x₁" and "x₂" are equal.

"x" and "x₁" each contain five atoms and four valleys but "x₂" contains nearly seven atoms and six valleys. Since the distances are equal the valleys must be shallower in the "x₂" direction.

Slip will occur, as indicated by the arrows, in the "x₂" direction. Even though a tensile force has been applied slip and eventual failure will be shear.
Figure 17 is a microphotograph of the polished surface of a sample of plastically deformed copper.

The slip planes can be seen as a series of roughly parallel lines across the central grain.

A second mechanism by which permanent deformation or dislocation occurs is by twinning.

**TWINNING:** Twinning can occur either:

1. By the application of a force to cause mechanical or strain twins or
2. During crystal regrowth after heating above the recrystallisation temperature and allowing to cool. These are called annealing twins.

**NOTE:** The recrystallisation temperature for a material is the temperature, above which the Kinetic Energy of the atoms is high enough to break down the bonding forces holding the atoms in the lattice structure.

Slip deformation occurs when planes of atoms are displaced so that the atoms take up new positions in the original crystal lattice. (See Figure 18).

![SLIP Diagram](Image)
Twinning dislocation is the result of atoms moving to positions which are not in the original space lattice.

Figure 19 shows the rearrangement of atoms to new positions which are not at the intersection of lines in the original lattice. The repositioning is such that the new crystals formed are symmetrical about the twin planes.

\[ \text{TWINNING} \]

![Diagram of twin formation](image)

**Fig. 19.**

Twinning occurs more readily in some materials than others. Of the commonly used metals iron, tin, zinc and copper are most susceptible to this form of deformation.

Narrow twins, called "Newmann Bands", readily form in iron at low temperature under shock loading. If a bar of tin is bent back and forth the formation of the twin crystals is accompanied by a distinctive "crackling" sound.

The micrograph (Figure 20[a]) shows twin crystals together with slip planes in a specimen (Mag. x 50). These are strain or mechanical twins.

Figure 20(b) shows the same specimen after annealing. The twin crystals were formed during grain growth and are annealing twins. The slip planes have disappeared.
Deformation due to both slip and twinning is limited to individual grains. When the grain boundary is reached the deformation is arrested and restarts either elsewhere in the same grain or in other grains.

In most cases the total deformation is a combination of slip and twinning.

In all cases final failure is due to slip, the twinning process rearranging the lattice structure to favour slip.

**STRAIN OR WORK HARDENING**

With the slip and twinning methods of plastic deformation the build-up of resistance to continued deformation is by the "clogging" of slip and twin planes. This is a very important characteristic of all industrially useful materials.

Without this build-up, which we call work hardening or strain hardening, materials would continue to slip and eventually fail as soon as the yield stress of the material was reached.

It is thought that the hardness and strength developed, as work hardening proceeds, results from the increasing difficulty in moving atom groups against the pile-up of already jammed slip and twin planes.

**PROPERTY CHANGES DUE TO WORK HARDENING**

The effect of work hardening on the properties of a metal are as follows:

**HARDNESS:** As the name implies there is a steady increase in hardness with the development of work hardening to the point of failure by fracture.

**DUCTILITY:** With the increase in work hardening there is a steady decrease in ductility. As ductility approaches zero failure due to brittleness occurs.
**STRENGTH:** Both tensile and yield strength increase steadily as work hardening develops.

**ELECTRICAL CONDUCTIVITY:** As a general rule there is decrease in conductivity with the development of work hardening.

The rate of decrease depends on the conductivity rate of the metal in its unworked state.

e.g. Steel has a relatively low rate of conductivity (compared to copper and aluminium) and the drop in conductivity of steel in the initial stages of work hardening is quite dramatic when compared with the better conductors.

The graph in Figure 21 illustrates the relationship between work hardening and electrical conductivity.

![Graph showing the relationship between electrical conductivity and work hardening for copper, aluminium, and steel.](image)

**Fig. 21.**

**ANNELING**

The effects of work hardening can be reversed by a process called annealing.

This involves the heating of the metal to above its recrystallisation temperature and allowing it to cool to room temperature.

The energy stored in a material during work hardening is dissipated by the rapid diffusion of the displaced atoms at high temperature. The displaced atoms resume their original lattice positions during recrystallisation. The material is then in an unstrained condition and the property changes due to work hardening have been reversed.

Annealing will be covered in more detail in a later Topic.
MECHANICAL PROPERTIES

Mechanical properties are those which are associated with a material's ability to resist or modify the effects of externally applied forces.

If a material is difficult to scratch we say it is hard, if it doesn't fail when large forces are applied we say it is strong, if it can absorb extensive plastic deformation without failure we say it is tough.

With a knowledge of these and other properties the engineer will be able to choose the most suitable material for the task at hand. Sometimes he will need a material which will not deform under load.

E.g. Bridge members should remain very close to their original design shape when loaded.

In other situations materials need to permanently deform readily.

E.g. Copper and aluminium for wire and aluminium can production.

In other circumstances the part may need to deform and recover repeatedly.

E.g. A car spring.

In the Topic on Bonding we looked at the bond forces which maintain atomic particles of materials in their own particular structures.

In this Topic we have covered the mechanisms by which external forces overcome the bond forces to give deformation and dislocation.

These were slip and twinning.

We will now look at the properties of materials which either allow or resist deformation and for convenience we will list them in three groups.

1. Minimum Deformation.
2. Temporary Deformation.
3. Permanent Deformation.

1. MINIMUM DEFORMATION

HARDNESS: The ability of a material to withstand surface penetration by scratching, abrasion or indentation. See Topic on Testing.

STIFFNESS: Is a measure of a material's ability to resist deformation or deflection under load. The Modulus of Stiffness, Modulus of Elasticity or Young's Modulus are measurements of this property.

2. TEMPORARY DEFORMATION

ELASTICITY: The ability of a material to recover its original shape after a deforming load has been removed.

ELASTIC STRENGTH: The maximum stress level a material can stand and still return to its original dimensions when the load is removed.
This occurs very close to the yield point of mild steel or an acceptable yield or proof stress for materials with no yield point. For a brittle material it is close to the ultimate or fracture strength.

**Resilience**: This is a material's ability to absorb and return applied energy without plastic deformation.

If the stress/strain diagram for a material is produced the area under the elastic part of the diagram is a measure of the Modulus of Resilience. (See Figure 22).

![Stress vs Strain Diagram](image)

*Fig. 22.*

The area OAB is a measure of the Modulus of Resilience of the mild steel sample.

High resilience materials have high yield strength and low Young's Modulus.

A spring is an example of a part possessing high levels of resilience.

Bear in mind that although a spring (or rubber) returns to its original dimensions when the load is removed it does not obey Hooke’s Law and hence there is no straight line part of the Stress/Strain diagram and no Young’s Modulus.

3. **Permanent Deformation**

**Ultimate Strength**: The maximum stress level the material can stand. After this stress level the sample develops necking and further deformation occurs at the neck. The stress level falls steadily to failure accompanied by large increases in strain.

Ductile materials display necking and Fracture Stress is always less than Ultimate Stress.
Brittle materials do not display necking and Fracture Stress is very close to Ultimate Stress.

TOUGHNESS: This is the amount of energy required to cause a material to fail.

Using the stress/strain diagram for the material the total area under the curve to failure is a measure of the material's toughness. It includes both elastic and plastic deformation. (See Figure 23).

The area OABC is a measure of the Toughness of the sample.

Figure 24 shows the stress/strain diagrams for a brittle and a ductile material of approximately equal strength (i.e. U.T.S. is the same).

It is clear that the ductile material is the Tougher of the two.

NOTE: Both Resilience and Toughness are related to energy and a value in Nm (J) can be obtained by calculating using readings from the stress/strain diagram, the amount of work done in deforming the sample.
SHEAR STRENGTH: Since most metals are weaker in shear than in tension, failure will occur along appropriate slip planes.

The component of the tensile stress which just produces slip along that slip plane is referred to as the Critical Shear Stress for the material.

Figure 25 shows how the tensile force $F$ can be resolved parallel to and normal to the slip plane direction.

The Critical Shear Stress value for this material will be:

$$\frac{F \cos \alpha \text{ MPa}}{A}$$

where $\alpha$ is the slip plane angle and $A$ is the C.S.A. of the piece.

$F \cos \alpha$

(Component of $F$ along slip plane)

Fig. 25.

NOTE: This is a simplified description since in most crystalline materials slip occurs in a number of directions. 3 unit work covers this area in more detail.