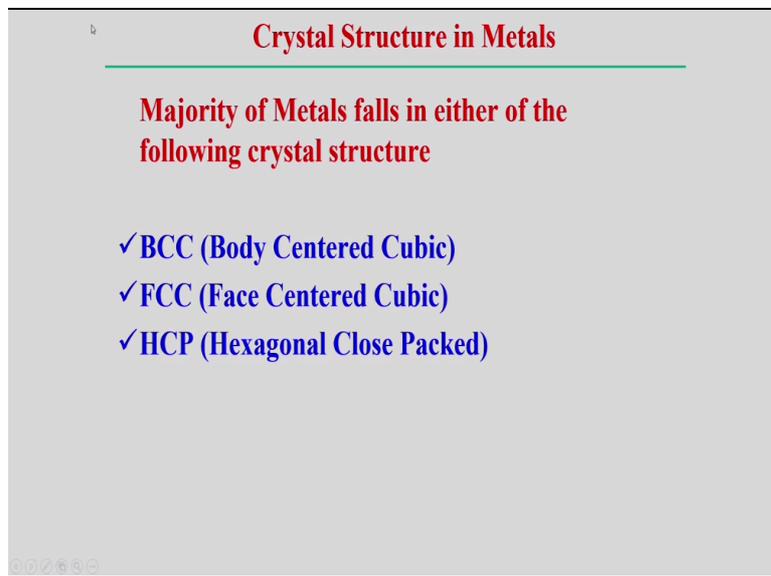


**Mathematical Modeling of Manufacturing Processes**  
**Swarup Bag**  
**Department of Mechanical Engineering**  
**Indian Institute of Technology, Guwahati**

**Lecture - 02**  
**Materials and Manufacturing Processes - 2**

Hi, we are trying to discussing the different types of the materials or actually if you look into the structure of the materials, we normally start with the crystal structure of the metals. Definitely, the crystal structure having some relation with the final properties even if you look into the properties in the macroscale then having some influence of the crystal structure to for a particular properties of a particular material.

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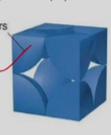
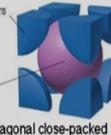
**Crystal Structure in Metals**

**Majority of Metals falls in either of the following crystal structure**

- ✓ BCC (Body Centered Cubic)
- ✓ FCC (Face Centered Cubic)
- ✓ HCP (Hexagonal Close Packed)

So, majority of the metals we use the engineering materials, in normal life we use that, that is the following 3 categories normally can found out that BCC, one is the body centered cubic structure, FCC structure face centered cubic structure and hexagonal close packed structure. Of course, there are other types of the crystal structure but these are the 3 types of the structures we normally explain in most of the engineering materials.

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Type of Packing	Packing Efficiency	Coordination Number
Simple cubic (sc) $\frac{1}{8}$ atom at 8 corners 	52%	6
Body-centered cubic (bcc) $\frac{1}{8}$ atom at 8 corners 1 atom at center 	68%	8
Hexagonal close-packed (hcp) Cubic close-packed (ccp or fcc) $\frac{1}{8}$ atom at 8 corners $\frac{1}{2}$ atom at 6 faces 	74%	12
$\text{HCP} = 12 \times \frac{1}{6} + 2 \times \frac{1}{2} + 3 = 6$		

Now, this is a different branch of study that in details about the crystal structure and then properties of a particular metal but we try to overall try to look into the what are the different types of the crystal structure normally explains. For example, if we represent the materials in the form of unit cell, sometimes all the characteristic arrangement of atoms can be represented within the unit cell.

Now, in that sense there are the properties depends on this all these measurable parameters. For example, number of atoms within the unit cell, what is the theoretical density, from here you can estimate the coordination number that means how one atom is linked with the neighboring atoms. So, based on that we can define the coordination number and of course how this relates between the atomic radius and the lattice parameter.

And of course, how densely the atoms are packed within the unit cell, all these parameters decides or represents some different particular type of the properties of these. For example, we know that this is first one is the simple cubic structure and this is one type of crystal structure and if you see that in the simple cubic structure all the corner atoms actually occupied and since unit cell representation that only one times out of the 8 actually taking the filling the volume of each corner point.

So, if we looking into the packing fraction or packing efficiency, how densely packed within the unit cell then it is getting only 52% volume is occupied by the atoms and of course in this cases how one atom is surrounded by the neighboring atoms that is based on that we get the

coordination number 6 and of course similarly if you look into that body centered cubic structure BCC structure.

Its packing fraction is more as compared to the simple cubic structure 68% here and coordination number actually 8 in this case and the atoms represented in such a way that in the body centered cubic means at the centre body there is one atom and the other atoms are just actually touching with the centre atom along the body diagonal. Similarly, if you look into the hexagonal close packed HCP structure; this is the typical structure of a HCP structure hexagonal close packed.

And other one is the cubic close packed structure or you can say that FCC structure face centered cubic structure. So, face centered cubic structure we see that here also both the cases the packing fraction is actually 74% and coordination of both the cases 12 but one represents the four axes system to represent that structure that is the hexagonal close packed structure and cubic close packed structure or FCC structure.

That we need the three axes system to represent the atomic arrangement all this things but I am not going into detail how to evaluate all these parameters and these things but overall if you look into that this total number of atoms within the unit cell, we can easily estimate total number of atoms within the unit cell I think for this is 1 and of course other cases there are different number of atoms within the unit cell.

But I think in case of HCP there are 6 atoms within the unit cell but that is one matter, apart from that how densely it pack within the unit cell and properties actually where is depending on that. So, here overall look into the different types of the crystal structure, we can say that these are the most densely packed HCP and FCC close packed structure as compared to the BCC structure.

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$$\rho_{\text{metal}} > \rho_{\text{ceramics}} > \rho_{\text{polymers}}$$

**Metals** - close-packing (metallic bonding) and large atomic mass

**Ceramics** - less dense packing (covalent bonding) and often lighter elements

**Polymers** - poor packing (often amorphous) and lighter elements (C, H, O)

**Composites** - intermediate values

Now, with this structural representation of the atoms, we can predict to some extent the properties. For example, here we try to look into that what are the properties for example first is the metals is the close pack structure and of course these atoms are connected through the metallic bonding and large atomic mass, this is a typical characteristic of a metal. Then, ceramics, we can see it is; here it is less densely packing and of course form the bonding between the atoms is the covalent bonding.

And of course, the elements consists of the lighter elements, so therefore if we compare between these two and we can see the density of the metal is normally more as compared to the ceramic material and of course all this depends on the what type of the crystal structure and what elements actually forms the crystals, based on that we can predict the property, so density is more as metal in case as compared to the ceramic.

If you look into the polymer also, the poor packing, packing of the atoms are not good in this case but often creates the amorphous structure and which is equivalent like kind of glass structure and lighter elements normally forms carbon, hydrogen and oxygen as compared to the metals. So, therefore polymer having in this cases the least density and of course composites have some intermediate value.

So purpose is to that by looking into the crystal structure if you know for a particular metals or whether it is polymer or ceramics, what type of atomic arrangement it follows and the crystal is from what type of atoms, so whether it is heavier atom or whether it is lighter atom.

The properties to density we can practically we can estimate what is the density of this particular materials by looking into their crystal structure.

Of course, if you know the FCC, BCC or HCP different types of the crystal structures, we can easily estimate what is the theoretical density of a particular metal that is also possible but by knowing the crystal structure, it is not always possible to predict the material properties at the microscale or at the continuum scale what are the mechanical properties is very difficult to predict because the material properties not only depends on the type of the crystal structure rather it depends on the other parameters.

For example, presence of defects within this crystals, what is the grain morphology, grain size, so all influence more and when we try to predict the bulk properties of a particular material rather than what is the crystal structure that means the lower prediction of a material properties at the higher scale by looking into the structure of the lower scale is sometimes difficult because intermediate we need to know other information.

So, just an example what is the average grain size, the distribution, presence of defects, presence of any second phase particles, all actually influence the mechanical properties of a particular material but just to up to certain extent we can predict the properties of a material just by looking into the crystal structure.

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**Physical properties**

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**Density:** Of a substance is its mass per unit volume ✓  
Mathematically: Density is mass divided by volume

$$\rho = \frac{m}{V}, \quad \checkmark$$

where  $\rho$  is the density,  $m$  is the mass, and  $V$  is the volume

**Melting point of a solid** - temperature at which the solid phase changes to liquid at atmospheric pressure

**Specific heat:** Energy required to change the temperature of an object by unit degree or Kelvin. ✓

Metals have lower specific heat capacity than plastics. To attain a particular temperature, **metal needs less heat energy than plastic**

Now, what are the physical properties normally measured for a particular material that we try to look into this thing not in manufacturing process in other process also. One is the density,

density is measured is mass per unit volume that we know, it can be represented  $\rho = m/V$  where  $m$  is the mass and  $V$  is the volume. If we know the mass and volume, we can easily estimate the density but density depends on the temperature also.

Then, these material properties also important; one is the melting point of particular solid, so temperature at which the solid phase transforms to the liquid phase that is we can say that is a melting point of a solid. So, this melting point normally in case of pure metal, the melting point is a fixed one single value but in case of alloy the melting happens over a range of temperature that is called between solidus temperature and liquidus temperature.

So that we can define the range of the melting for an alloy system. Then, specific heat is other type of the metal properties, so specific heat we can define the energy required to change the temperature of an object per unit degree that we know that what is the energy required just to change component for single degree either degree centigrade or Kelvin. So, normally metals having the high specific heat as compared to the plastics.

Therefore, to attain the particular temperature, we need metal needs less amount of heat energy as compared to the plastic. So, that kind of information is by looking into the properties of the specific heat.

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**Physical properties**

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**Thermal conductivity:** Property of a material to conduct heat flow

**High thermal conductivity material** – Copper, Aluminum, Silver, Gold

**Materials with low thermal conductance** – Polymer, alumina – can be used for insulation purpose

**Thermal expansion** - Change in volume in response to change in temperature

- ✓ Creates thermal strain in solid
- ✓ Degree of expansion per unit change in temperature is called the material's **coefficient of thermal expansion**
- ✓ However, it varies with temperature

$\alpha = \frac{1}{\Delta T}$   
 $\alpha(T) = ?$

Then thermal conductivity property of a material to conduct the heat flow. That is the measurement of a thermal conductivity for a particular material. So, normally you know the copper, aluminium, gold, silver that is having very high thermal conductivity. So, they

transfer the heat very quickly as compared to the other as compared to the for example steel and that is the difference whether that this properties of different.

This thermal property is different between the steel and the other type of the metals like copper, aluminium or silver and gold. So, metal is the low thermal conductance for example polymer, alumina, kind of ceramic polymer, they are having very low thermal conductivity or sometimes polymer can be used as a thermal insulation not having any thermal conductivity as well. So, sometimes used for the insulation purpose.

So, similarly other properties that is called thermal expansion, the change of volume in response to the temperature. If there is a change of the temperature, how it changes in the particular volume or maybe in particular direction what is a linear change of a particular system with respect to change in the temperature. That is a measure of the thermal expansion that means expansion due to the application of the temperature difference or application of the heat energy.

But of course, this heat energy distributes uniformly or if there maybe if it is free to move that particular material then it may not create any kind of the stress but when it is restricting the movement of the particular solid even there is a change of the temperature then it can create kind of the stresses within that body. So, change in the thermal expansion actually related to the change in thermal strain in solid.

So, thermal expansion creates the thermal strain, of course thermal strain will be created if we restrict the movement during the application of the thermal energy to particular. So, degree of expansion per unit change in temperature is called the material's coefficient of the thermal expansion. Coefficient of thermal expansion normally measure the dimensions per unit degree centigrade or per Kelvin, change in 1 Kelvin.

So, therefore this is the coefficient of thermal expansion, we can measure it that however, it varies with temperature. So, even coefficient of thermal expansion actually is a function of temperature, so it varies depending upon, at different temperature the coefficients of thermal expansion are different.

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## Mechanical properties

**Strain( $\epsilon$ ):** Change in dimension per unit original dimension

**Stress ( $\sigma$  or  $\tau$ ):** Applied force per unit area

$$\frac{dl}{l} = \epsilon$$

**Normal Stress and Shear stress**

**Strength:** Ability of a material to resist the applied force without breaking or yielding.

**Stiffness:** Ability of material to resist deformation under stress

**Elasticity:** Property of material to regain its original shape after deformation when the external force are removed

Steel is more elastic than rubber

**Plasticity:** Property of a material which retains permanent deformation with the applied load

Then, other mechanical properties, other properties is that strain, change in dimension per unit original dimension. So, change in dimension  $dl$  and with respect to original dimension that we can measure the strain and we can see the strain is dimensionless quantity here and stress we can measure that applied force per unit area. So, applied force per unit area but stress can be normal, stress can be shear stress also.

When we estimate the normal stress, we consider that area perpendicular to the applied force but when you estimate the shear stress then we need to consider the area which is parallel to the applied force so that force divided by that area represents the shear stress or normal stress depending upon the which direction load is acting. Then, strength of a material can be defined the ability of material to resist the applied force without breaking or yielding.

So, before breaking and yielding what are the amount of the force this can absorb, then that that is a measure of strength of a particular material. Similarly stiffness, stiffness is the measurement, ability of material to resist the deformation under application of the stress that is a measure of the stiffness for a particular material. Apart from that other mechanical properties the elasticity is the one kind of property.

Property of a material to regain its original shape after deformation that means if we deform one particular material and after certain point if you remove the load and if it come back to the original position, then that is called the elastic properties of a particular material but what is the maximum below the before the yielding starts up to that point the material behaves

elastically and once it crossed the yield point normally metals behaves as plastic when it enters the plastic zone, then permanent deformation exist.

So, therefore plasticity of a material which remains which retains the permanent deformation so, therefore even we remove the load if there is after permanent deformation particular material then the material will not come back to the initial position. So, that means we can say that some plastic deformation happens within the application of the load for a particular material, so that is why we can differentiate between elasticity and plasticity.

These are the typical properties of a material we need to consider during the simulation process.

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**Mechanical properties**

**Ductility:** Ability of a material enabling it to be drawn in to wire with the application of a tensile force

**Brittleness:** It is property of a material opposite to ductility.  
Cast iron is a brittle material

**Malleability:** Special case of ductility which permits materials to be rolled or hammered in to thin sheets.  
Ex. aluminum ✓

**Toughness:** Property of material to resist fracture due to high impact load  
Measurement - Energy absorbed before fracture ✓

**Resilience:** Amount of energy when deformed elastically and release upon unloading

Then, ductility, ductility means ability of a material to enable to drawn in a particular, drawn into the wire with application of the tensile force, how much deformation it can absorb that is called that is a measure of the ductility and brittleness is just opposite to the ductility that means with application of the load, material breaks without much deformation. Then, we can say that is the brittleness that is because of the brittleness properties of the material.

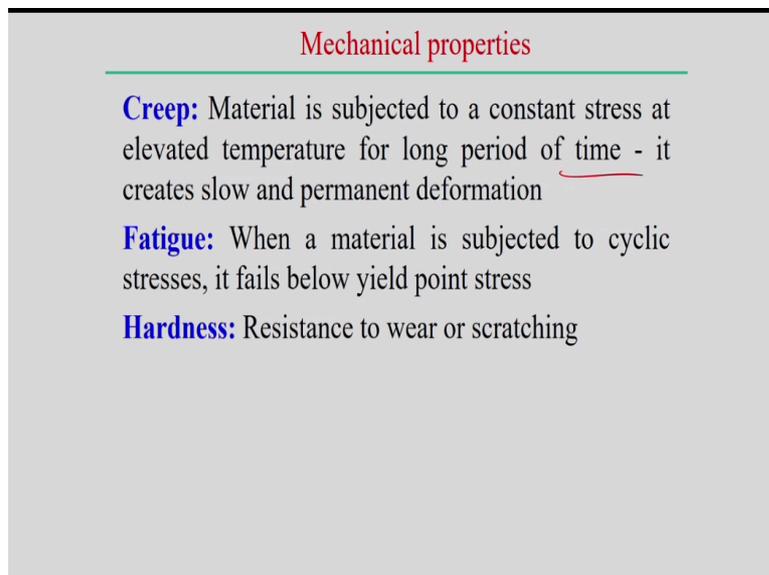
For example, cast iron is the brittle material as compared to the mild steel for example. So, mild steel is we can say the ductile material but cast iron we can say is the brittle material. Malleability means the special case of the ductility which permits the materials to be rolled or hammered into the very thin sheet. If materials can easily form with application the load is a very thin sheet.

Then, we can say the malleability is a property that is responsible to make a very thin sheet with application of the load for example, aluminium having good malleability property. Similarly, toughness we can measure the amount of energy absorbed before fracture, so that is the measure of the property of the material to resist the fracture due to the high impact load. So, measurement so energy absorbed before fracture that is the measurement of the toughness.

So, toughness is simply we can measure in terms of what is the amount of the energy absorbed before the fracture. Resilience, amount of energy when that is deformed up to the elastic point and released upon the unloading, so, resilience can be measures what is the amount of the energy up to the yield point. So, just below or we can say just below the yield what is the amount of energy can we absorb.

That means once we remove the load the unloading that amount of the energy can be released. So, that is the measurement of the resilience of a particular material.

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**Mechanical properties**

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**Creep:** Material is subjected to a constant stress at elevated temperature for long period of time - it creates slow and permanent deformation

**Fatigue:** When a material is subjected to cyclic stresses, it fails below yield point stress

**Hardness:** Resistance to wear or scratching

So, these are the typical properties apart from that the creep property also we can measure sometimes required and that creep property is mainly significant relatively at very high temperature not in the ambient temperature. So, we can define the creep like that material is subjected to a constant stress at elevated temperature for a long period of time. So, therefore it creates the slow and permanent deformation, slow and permanent deformation is created because of the creep property.

So, therefore creep property is the properties which is significant the conditions at very high temperature and at high temperature when metal is subjected to some kind of the constant load, till with the application the constant load some amount of the deformation normally happens, so that is the creep properties of a particular material. Then, fatigue is one of the properties of a particular metal.

That is when the metal is not subjected to very kind of static loading condition and this is a dynamic loading conditions or cyclic stresses or cyclic loading condition that such that it creates the cyclic stresses. So, under that kind of loading condition, the material may fail before reaching the yield point.

So, that is the measure of the fatigue properties but of course when we measure the fatigue properties of a particular material, what is the loading pattern is important here. So, that means cyclic loading pattern, what is the change in the state from say tensile to compressive and second point is that up to what number of cycles, what are the failure stress, based on that we can decide the fatigue properties of a particular material.

And hardness is normally we use any kind of experiment, we measure the hardness distribution of a particular component but hardness is resistance to wear or scratching that resist to wear or scratching to represent these things. So, all these properties, mechanical properties as well as physical properties are actually significant to know and we frequently use all kind of properties.

And the different types of the problem and this problem in the sense the different types of the manufacturing process and of course when we try to analyze any manufacture component, we normally to go through all this kind of the, to evaluate all this kind of the mechanical properties and based on these properties, the application area can be decided.

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**Other properties**

- ✓ Latent Heat of Material, Thermal diffusivity →  $\alpha = \frac{k}{\rho c_p}$
- ✓ Viscosity →  $\sim \frac{m^2}{s}$
- ✓ Electrical conductivity, Electrical resistivity
- ✓ Magnetic properties – induction welding

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- ✓ In machining, welding, casting - thermal properties of the work is important
- ✓ Casting and welding – Fluid property is significant
- ✓ Semiconductor manufacturing - electrical properties of silicon is important
- ✓ Mass diffusion coefficient – surface hardening or diffusion welding

$H = \rho c_p t$

Now, other properties also exist in case of manufacturing processes that is called the latent heat of material that we need to understand, latent heat of material like we can estimate there is in case of water there is change of the phase from liquid phase to solid phase but it is accounted at a particular fixed temperature, some amount of heat energy absorbed. So, similar thing happens in case of metals also.

So, metals also subjected to some amount of the latent heat when there is a change of the phase from one phase to another phase, say solid phase to normally solid phase to liquid phase, it is account to that but this phase change happens in case of pure metal at constant temperature. So, that is latent heat of material is basically important during the solidification process as well or during the welding process or casting process.

And another material property we normally estimate the use thermal diffusivity that means what is the rate of the heat penetration for a particular material. So, thermal diffusivity can be represented by  $k/\rho c_p$ , it is a combination of the properties that means  $k$  is the thermal conductivity of a particular material,  $c$  is the specific heat,  $c_p$  is the specific heat and  $\rho$  is the density. So, in SI unit the unit is meter square per second.

So, that is the measure of the thermal diffusivity of a particular material in terms of other parameters. Similarly, viscosity is the property but viscosity in manufacturing process is required and we need to analyze the flow analysis, flow analysis may be associated with the casting process or may be associated with the small whirlpool, when you do analysis of the fluid flow in that cases the viscous properties is important.

So, therefore viscosity is another property which can be usable during the simulation of the manufacturing processes. So, of course electrical conductivity and electrical resistivity that process which involved. For example, resistance, spot welding process. There the electrical resistivity is also important because that electrical resistivity is a simply resistance to the flow of the current and that actually create some amount of heat generation.

And based on that principle  $H=I^2 R t$  so R is the resistance here, so just measuring the resistance during the spot welding process we can estimate the heat generation. Therefore, electrical resistivity also another parameter we need to incorporate, we need to know in manufacturing processes. Of course, magnetic properties also because magnetic we need to develop some kind of induction welding process.

So, in that cases the magnetic properties of a particular metal is useful. So, all this apart from all these material properties we have already discussed, all this other type of material properties is also significant when you try to look into the, try to analyze the different manufacturing processes by just looking into this thing. This is just overview of different types of the properties.

Now, if you look into the different manufacturing processes, first we look in the machining process, machining, welding and casting. All these cases, if we do heat transfer analysis, then thermal properties of the workpiece is more important because all element to the properties are of course we can do, in welding and casting the fluid flow analysis also, then viscous flow for this also important in this cases.

Then, casting and welding; casting and welding of course here the fluid property is significant, we need to look into that type of analysis and what are the material properties actually involve this type of analysis. Definitely, when you try to make develop some kind of the model, we need to define first what are the metal properties are required to explain the physical model and based on that we give the input, the value of this material properties.

And of course, these material properties are normally evaluated experimentally. Then, semiconductor manufacturing, so in semiconductor manufacturing we try to model or in the manufacturing process we try to analyze this process, electrical properties of the silicon is

important there, so therefore we look into all the electrical properties of particular component and in semiconductor manufacturing.

Definitely, mass diffusion coefficients; so mass diffusion coefficients another type of the properties we can define but this mass diffusion coefficient is significant in case of the surface hardening or diffusion welding and surface hardening and diffusion welding how the heat is diffused during this process. So, then or this atomic diffusion happens within this particular material.

In those cases, the diffusion coefficient is more significant to define. So, therefore if you look into different analysis, there are different types of properties and we need to know what properties is important in what type of manufacturing processes. So, I hope with this analysis of the different type of the properties, we can get some idea that what are the properties, what is the role of these properties to analyze of a particular manufacturing processes. So, thank you very much for your kind attention.