Introduction to crystal elasticity and crystal plasticity

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Week-01
Lecture-01

Hello everybody; myself Swarup Bag. So I'm considering this time on mock course introduction to crystal elasticity and crystal plasticity. So basically I am a faculty member so presently as (ass) Assistant Professor at the Department of mechanical engineering, IIT, Guwahati. So my area of work is basically manufacturing and materials. So very specifically focused on the manufacturing processes and that processes generally link to the properties of the manufactured product.

So I taught in the last few semester the courses like engineering materials manifesting technology and also what is a tutorial in the engineering mechanics course. So such type of basic courses at the same time Masters courses like physics of manufacturing processes. So my area of research work is basically the focused on the welding and joining technologies and different mathematical approach linking to the different skills of analysis to produce the practically multiskilled approach and it is very specific to the manufacturing processes.

So these courses like introduction to (class) crystal elasticity and crystal plasticity is a (part one) a part of the course that currently I am involved in the, this (sp) specific research area. So this courses; hopefully it will be enjoyable to you so my objective in this course to produce very simplified way so that very beginners can learn this course without much struggle, without much background of the subject itself. So focus of this course is specifically the elasticity and plasticity part for single crystal structure as well as poly crystalline structure and of course it is very specific to the metals and alloy.

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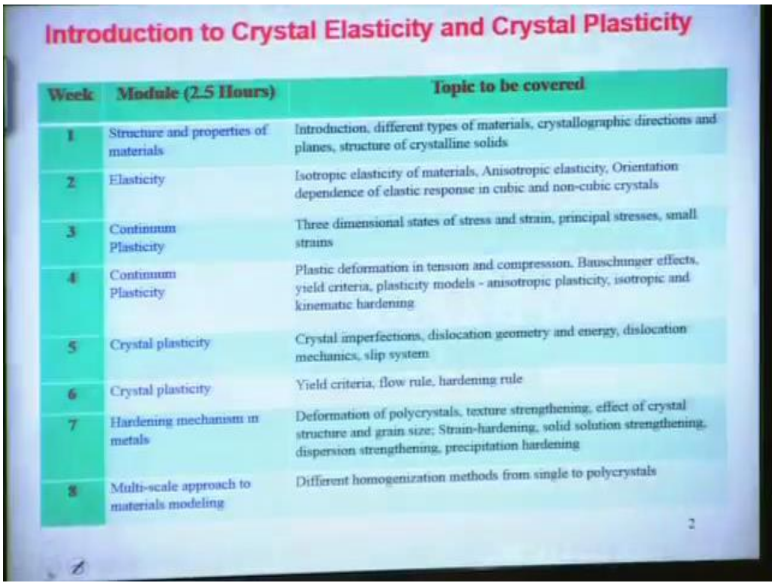

Introduction to Crystal Elasticity and Crystal Plasticity

Week	Module (2.5 Hours)	Topic to be covered
1	Structure and properties of materials	Introduction, different types of materials, crystallographic directions and planes, structure of crystalline solids
2	Elasticity	Isotropic elasticity of materials, Anisotropic elasticity, Orientation dependence of elastic response in cubic and non-cubic crystals
3	Continuum Plasticity	Three dimensional states of stress and strain, principal stresses, small strains
4	Continuum Plasticity	Plastic deformation in tension and compression, Bauschinger effects, yield criteria, plasticity models - anisotropic plasticity, isotropic and kinematic hardening
5	Crystal plasticity	Crystal imperfections, dislocation geometry and energy, dislocation mechanics, slip system
6	Crystal plasticity	Yield criteria, flow rule, hardening rule
7	Hardening mechanism in metals	Deformation of polycrystals, texture strengthening, effect of crystal structure and grain size; Strain-hardening, solid solution strengthening, dispersion strengthening, precipitation hardening
8	Multi-scale approach to materials modeling	Different homogenization methods from single to polycrystals

So if you look into that different modules of this course and what are the different topics I like to cover in this course first on the very basics part which is structure and properties of the materials. So specifically first I'll start with the different type of materials, their crystalline structure and very specific toward crystallographic directions and the planes because this will be very much useful to further analysis (of on) in the ground of elasticity and plasticity for specific materials.

So next module will be the elasticity, so it is related to the plasticity of the single crystal had we tried to focus on the anisotropic properties of the single crystal structure and we will try to derive the orientation dependence of the Young's modulus and their elastic response specific to the crystal and (non) cubic and non-cubic crystals

Next, third module will be the continuum plasticity so here we will try to focus on the like strength of material courses basic three-dimensional state of the stresses and how we can derive the principal stresses and what is the importance of the small strain deformation in case of continuum plasticity. So next will be a continuation of the plasticity but the (be) behaviour of the material (as) as a bulk material during the plastic deformation process and considering the effect of the Bauschinger effect, yield criteria how can evaluate or how the yield surface (evo) evolve depending upon the yield criteria. And of course in this case we will try to consider the anisotropic (pla m) plasticity and we will cover the isotropic and kinematic hardening that is generally used for different (s) materials (mod) modelling of a different type of materials.

Next focus will be the crystal plasticity, in this case first we will start with the basic crystal structure, crystal imperfection, different dislocation geometry, (en) how to estimate the energy for different type of crystal defects, what are the slip mechanisms, how we can found out the yield criteria and flow rule, different type of (hardening) hardening rule we can form in case of single (crys) crystal structure.

Next finally the different type of hardening mechanisms like deformation of poly crystals, structure strengthening, different type of crystal (st) crystal structure and the grade site, strain hardening effect, solid solution strengthening, dispersion strengthening and the precipitation hardening. And finally we will try to link the different scales of approach through multi-skills modelling approach and in case of numerical modelling (of) numerical modelling of materials due to the application of the mechanical load to a specific material.

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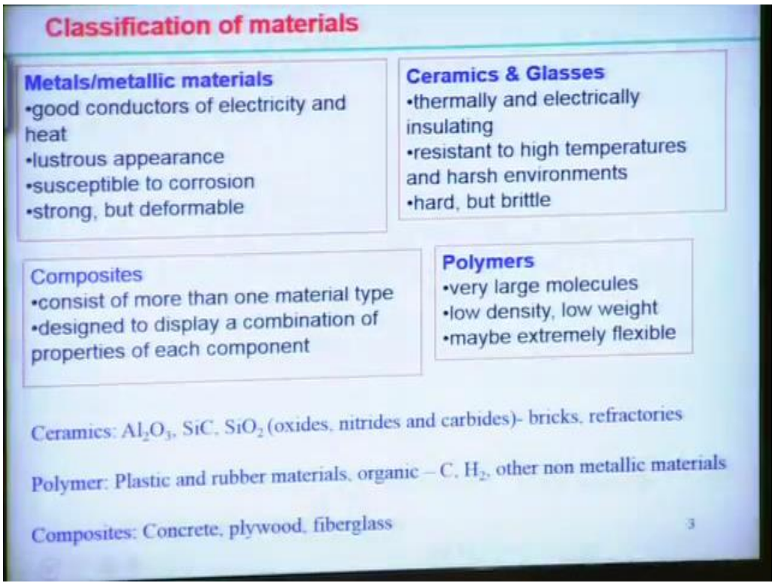

Classification of materials

Metals/metallic materials
- good conductors of electricity and heat
- lustrous appearance
- susceptible to corrosion
- strong, but deformable

Ceramics & Glasses
- thermally and electrically insulating
- resistant to high temperatures and harsh environments
- hard, but brittle

Composites
- consist of more than one material type
- designed to display a combination of properties of each component

Polymers
- very large molecules
- low density, low weight
- maybe extremely flexible

Ceramics: Al_2O_3, SiC, SiO_2 (oxides, nitrides and carbides)- bricks, refractories

Polymer: Plastic and rubber materials, organic – C, H_2, other non metallic materials

Composites: Concrete, plywood, fiberglass

So next we will try to come back to the very basic classification of different materials (jon) normally could be used for the engineering applications. So it is a very, classified materials in the 4 categorisation; first is the metals and metallic materials, ceramic and glasses, composites and polymers; these are the 4 types of materials normally used in our daily life. So as you know that the metals or metallic materials is basically we know that it is a good conductors of electricity as well as heat also. And it is also susceptible to the corrosion, it is very strong or maybe at the same time it may be deformable. So this is the common categorisation of the metals and different (met) metals and their alloy also.

And ceramics also thermally and electrically insulated material generally considered as ceramics material which is having very high resistance to (high) resistance to high temperature as well as it is very hard but brittle. So several applications of the ceramic materials we generally find out which is mainly consists of the oxides, nitrites or carbides (and) and is a mixing form of the metals and non-metals like aluminium oxide, Silicon Carbide, Silicon oxides and bricks and refractories can also be considered as a ceramic materials.

Then we come to the different type of polymer materials which is basic polymers materials having generally very large molecules of chain having low-density, normally having low weight and maybe very much flexible. So polymers a generally categorisation as plastic and rubber materials and this organic materials consists of carbon and hydrogen forming different chains of molecules as well as other non-metallic materials can be involved to the form of the polymers.

Now we come to that composites. Composites actually consists of more than one type of material but it is designed to display a combination of 2 different type of materials but it is completely different from the oxides like aluminium oxide and Silicon Carbide. So basic objective of using the composites is to retain the use of the properties of both the materials. The examples of composites is like concrete, plywood and fibreglass. So nowadays it is a very much we found a lot of applications of the composites (eh ha) materials and the in the different manufacturing sectors.

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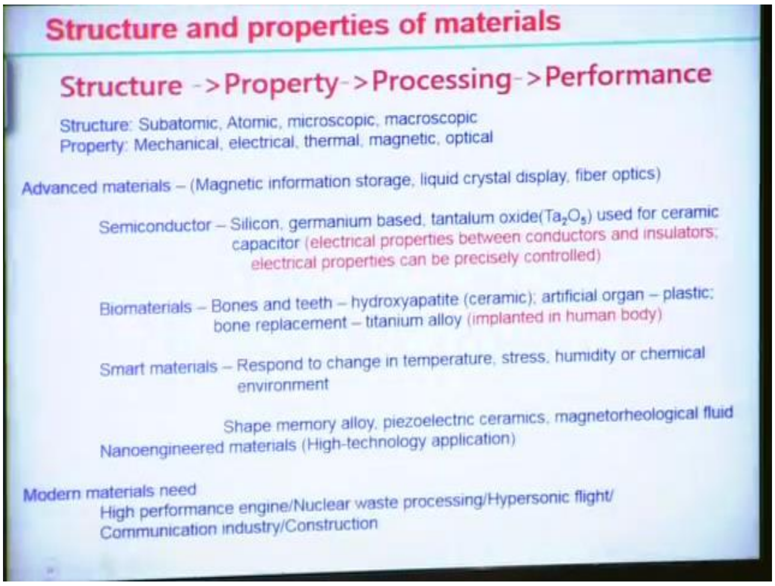

Structure and properties of materials

Structure ->Property->Processing->Performance

Structure: Subatomic, Atomic, microscopic, macroscopic
Property: Mechanical, electrical, thermal, magnetic, optical

Advanced materials – (Magnetic information storage, liquid crystal display, fiber optics)

Semiconductor – Silicon, germanium based, tantalum oxide(Ta_2O_5) used for ceramic capacitor (electrical properties between conductors and insulators; electrical properties can be precisely controlled)

Biomaterials – Bones and teeth – hydroxyapatite (ceramic); artificial organ – plastic; bone replacement – titanium alloy (implanted in human body)

Smart materials – Respond to change in temperature, stress, humidity or chemical environment

Shape memory alloy, piezoelectric ceramics, magnetorheological fluid

Nanoengineered materials (High-technology application)

Modern materials need
High performance engine/Nuclear waste processing/Hypersonic flight/
Communication industry/Construction

So (wh) what is the most interesting part of an engineer because, is that to know the structure, property, processing and the final performance of a specific materials. So this is a common chain kind of thing that always we are interested to performance of the specific material when it is subjected to some (kind) kind of environment or some kind of applied flow. But to understand the performance we need to the co-relation between the structure of different materials what are the properties and how we can process it and then as a result we can analyse the performance of a specific material.

So structure of a material starts from the subatomic, then atomic, microscopic, macroscopic; these are the different (s s) length of the scales where we can (built buil) builds the block or accordingly to find, to analyse the specific structure of a materials. So specifically the difference between the different length scale of the structure is the only in terms of nanometre range or maybe millimetre range.

For example subatomic structure can be considered if the length scale is less than 1 nanometre, maybe atomic scale can be considered, the length scale is less than 10 nanometre and microscopic can be 100 to 1000 nanometre, or macroscopic can be considered the length scale part it is more than 1 millimetre. So linking all this thing is basically the approach to a specific multiscale when we try to analyse as a whole the performance of the material and while we try to link it to the structure of material.

So now next to the structure is the property of a material, so maybe different type of material properties we can observe the mechanical, electrical, thermal, magnetic, optical that may have some practical importance to know.

Next is the processing of the materials; there are several manufacturing technologies exist to process the materials but to adopt for specific manufacturing process we need to know the property of a specific material. And finally the performance of the material (specific) which is very specific to application needed. Then we can analyse the performance of a material but before that we need to know what type of processing can be done for a specific material.

So nowadays there are several advancement of the metals also occurring continuously and what we can categorise is that different type of advanced materials like the magnetic information storage, liquid crystal display, fibre optics; these are the common advanced materials nowadays a lot of use can also be found for this advanced materials.

Other advanced materials is the semiconductor, there is a semiconductor, means the electrical properties actually vary, lies between the conductors and insulators. But the electrical properties can be very much precisely controlled in case of the semiconductor material. Silicon, germanium-based, tantalum oxide (and) these are (cap) used for the ceramic capacitor. So these are the typical semiconductor materials.

And nowadays there is a tremendous application of the advanced materials in (bio) bio related issues. So specifically that is called the biomaterials. So biomaterials is the (s un) first criteria of using any biomaterials is that it should be comfortable with the human body. So Bones and teeth, that is one kind of ceramic material, can be used as a biomaterial, artificial organ can nowadays can be produced using the plastic materials, bone replacement can be done, titanium alloy because all these alloys is very much sensitive to the bio environment.

Next is the smart materials. So nowadays (smart) smart materials is used in actuator where the smart material is specifically designed to respond to change in a specific environment; that environment can be the temperature, stress, humidity or some kind of chemical environment. So shape memory alloy which is specifically made of specific combination of nickel titanium, (like) nowadays is used, piezoelectric ceramics or the sense scans comes from the applied load or applied stress. And output can be captured using some input like stress or temperature change in case of smart materials.

So (())(14:46) also happening in case of (magneto) sorry nano engineered materials and the performance of the materials can be enhanced using the nano forming components in specific materials. However the needs of the, now in this society for more advanced material which is specifically (apply) applicable to the high-performance engine although (the) certain material a continuous development of the metals is going on, but till there is a need to specific material in case of high-performance engine (())(15:30) is the most important criteria as well as high heat resistance properties.

Nuclear waste processing now is also challenged there also we need some development of the materials to meet that kind of challenge. Hypersonic flight, communication industry, lot of atmospheres also happens using the modern advanced materials but till we need to do address for the development of the materials for this typical area.

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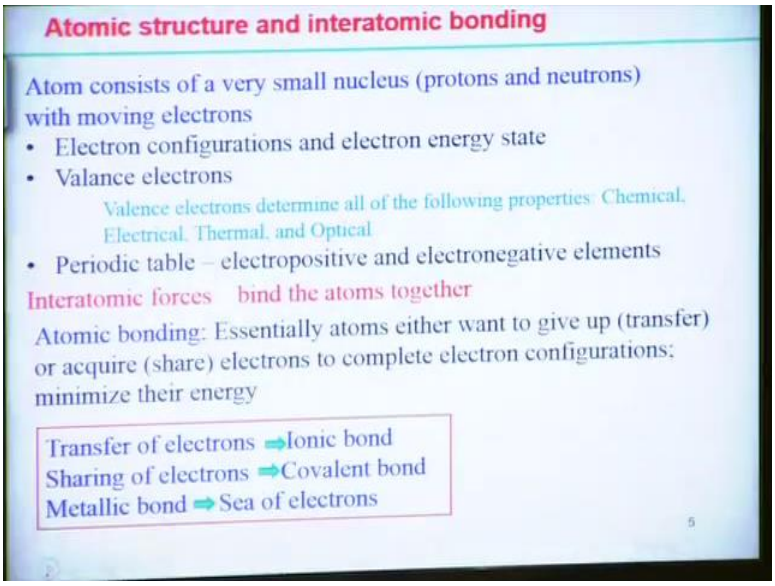

Atomic structure and interatomic bonding

Atom consists of a very small nucleus (protons and neutrons) with moving electrons

- Electron configurations and electron energy state
- Valance electrons

  Valence electrons determine all of the following properties: Chemical, Electrical, Thermal, and Optical
- Periodic table – electropositive and electronegative elements

Interatomic forces bind the atoms together

Atomic bonding: Essentially atoms either want to give up (transfer) or acquire (share) electrons to complete electron configurations: minimize their energy

Transfer of electrons ⇒Ionic bond
Sharing of electrons ⇒Covalent bond
Metallic bond ⇒Sea of electrons

Now we come to the very basic part of the structure. So, as we discussed the structure starts from the subatomic, atomic level crystal structure and then macroscopic and microscopic level, but we can start from the very beginning that is called atomic structure of a specific nature and interatomic bonding before start of the crystal structure of material. Now it is a well-known fact that atoms consist of the very small (s) nucleus and within the nucleus, protons and neutron exist but outer cell, there is existence of the electron. This is a typical structure of the atoms.

But the properties actually depend on the electronic configuration and the energy state of the, state level of the electron for a specific material. But here the valance electrons can influence the properties of the materials like chemical, electrical, thermal and optical properties is largely determined by the valance electrons. Of course there is a several elements exist and all these elements are arranged (in) in the periodic table depending upon the specific configuration that is the electropositivity or electronegativity of the elements. So this is a very use of the, (m) use to identify the specific properties of a material while we try to look into the atomic structure of a material, okay?

But existence of the (atomic) atoms depends on the how they are binding together that is called the interatomic forces.

Normally, there are several type of interatomic forces and that binds the atoms together and they also influence the properties of a specific material. So atomic bonding, essentially atoms always try to give up or acquire some amount of the electrons to complete their electron configurations and try to minimise the energy level. Based on this principle there are several bonding can be observed in case of atomic structure. Although it is very documented, I am trying to giving some overview of this kind of structure.

So transfer of electrons which is associated with the ionic bond and when there is a sharing of the electrons it is associated with the covalent bond, but metallic bond is associated with a sea of electrons. So all this 3 kind of bonds generally find out of the materials. There is another bond that is called secondary bond; that we will be discussing later on. So now we will try to focus on the interatomic bonding that is the ionic bonding.

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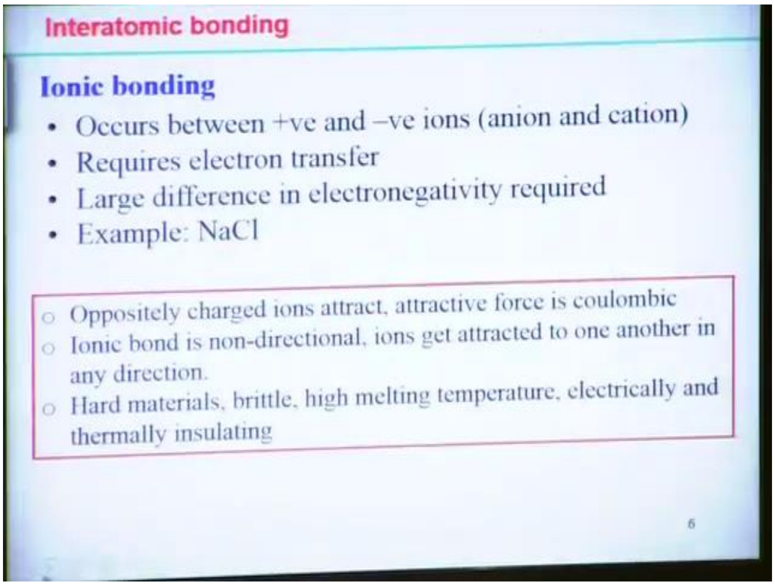

Interatomic bonding

Ionic bonding

- Occurs between +ve and –ve ions (anion and cation)
- Requires electron transfer
- Large difference in electronegativity required
- Example: NaCl

○ Oppositely charged ions attract, attractive force is coulombic
○ Ionic bond is non-directional, ions get attracted to one another in any direction.
○ Hard materials, brittle, high melting temperature, electrically and thermally insulating

So I need bonding occurs between positive and negative ions that is called cation and anion but it requires the (el) anyhow it requires the electron transfer. Large difference in electronegativity actually promotes the ionic bonding between the materials. One such example is that sodium chloride. So but what are the typical characteristic of ionic bonding is that it is oppositely charged ion attract and attractive force is coulombic force. But in case of ionic bonding it is non-directional. Ions get attracted to one another in any direction. Normally hard materials, brittle materials, high melting temperature materials, and electrically and thermally insulating materials we observe the ionic bonding between the atoms or ions.

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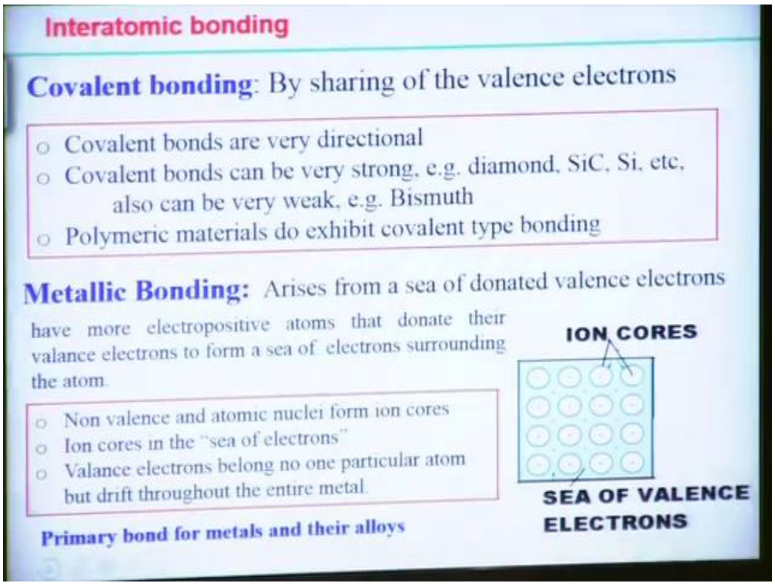

Interatomic bonding

Covalent bonding: By sharing of the valence electrons

- Covalent bonds are very directional
- Covalent bonds can be very strong, e.g. diamond, SiC, Si, etc, also can be very weak, e.g. Bismuth
- Polymeric materials do exhibit covalent type bonding

Metallic Bonding: Arises from a sea of donated valence electrons

have more electropositive atoms that donate their valance electrons to form a sea of electrons surrounding the atom.

- Non valence and atomic nuclei form ion cores
- Ion cores in the "sea of electrons"
- Valance electrons belong no one particular atom but drift throughout the entire metal.

Primary bond for metals and their alloys

Now we come to that point, the covalent bonding. The basic mechanism of covalent bonding is the share of the electrons. In this case the bonds becomes directional, which is not in the case of ion bonding, right? Covalent bondings can be very strong as well as it may be very weak also. For example Diamond, Silicon Carbide, Silicon having very good it is a very strong material but it is having covalent bond but at the same time Bismuth also it is very weak but it is also associated with the covalent bonds.

So, polymeric materials generally exhibit the different type of covalent bonding. Metallic bonding, as I told, it is associated with the sea of electrons and the having more electropositive atoms that donate their valance electrons to form sea of electrons surrounding the atom. So in this case, non-valance and the atomic nuclei actually form the ion cores. And valance electrons belong to no one particular atom but drift throughout the entire metal. Primary bond for metals and their alloy is generally follow the metallic bonding.

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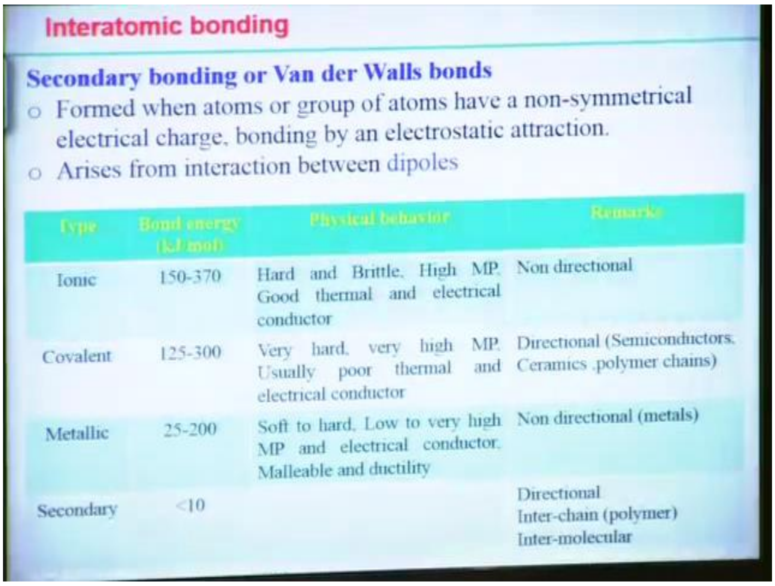

Interatomic bonding

Secondary bonding or Van der Walls bonds

- Formed when atoms or group of atoms have a non-symmetrical electrical charge, bonding by an electrostatic attraction.
- Arises from interaction between dipoles

Type	Bond energy (kJ/mol)	Physical behavior	Remarks
Ionic	150-370	Hard and Brittle, High MP. Good thermal and electrical conductor	Non directional
Covalent	125-300	Very hard, very high MP. Usually poor thermal and electrical conductor	Directional (Semiconductors, Ceramics ,polymer chains)
Metallic	25-200	Soft to hard, Low to very high MP and electrical conductor. Malleable and ductility	Non directional (metals)
Secondary	<10		Directional Inter-chain (polymer) Inter-molecular

Apart from the primary bonds there is also secondary bonding which is also called Van der Walls bonds. While different group of atoms have a non-symmetrical electrical charge, they actually (fo) they actually bond by the electrostatic attractions, and this arises actually from the interaction between the dipoles. Normally Van der Walls bonds are very weak as compared to the other primary bonds.

Now if we look into the summary of all different type of bonds and their specific remarks or conclusion from the different type of primary and secondary bonds. So, ionic bond; it is the bond energy roughly between the 150 to 370 kilojoule per mole but physical behaviour we observe in case of ionic bonding, it is typically hard and brittle, high melting point, could thermal and electrical conductor. But it is the nondirectional. Covalent bond, also similar range of the bond energy but it is very hard, it can be very high melting point temperature but usually poor in thermal and electrical conductor.

But difference is that from the ionic bonding is it is directional. So, semiconductor, ceramics and polymer chains generally observe this kind of covalent bonding. Metallic bond having very low bond energy as well as moderate energy which is 200 kilojoule per mole but it can be very soft, it can be very hard also having as well as low as well as very high melting point, having good electrical conductivity, also very good mechanical (conduct) mechanical properties like malleability and ductility.

But metallic bond is non-directional in nature and most of the metals will form the metallic bond. Secondary bond which is having very less amount of the bond energy as compared to the other 3 bonds, but it is directional; it form the inter-chain, inter-molecular and specifically polymer is having (the) this kind of secondary bonds. So this is all about the atomic structure.

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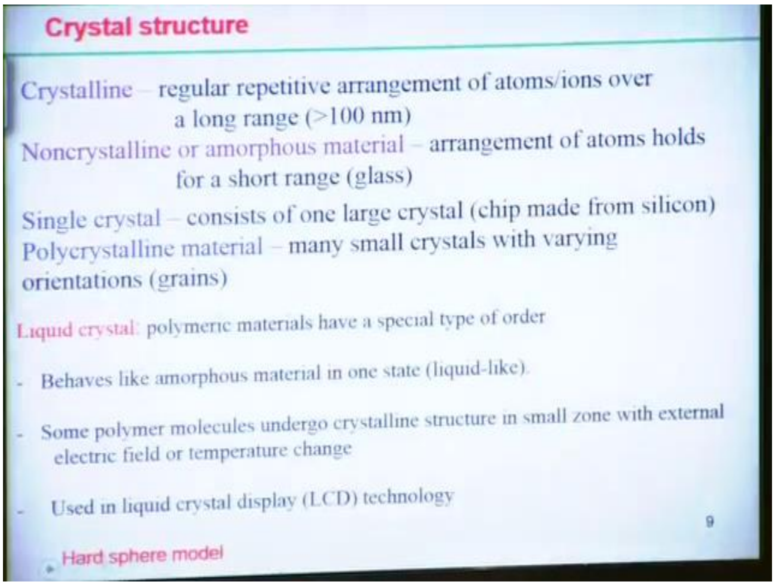

Crystal structure

Crystalline – regular repetitive arrangement of atoms/ions over a long range (>100 nm)

Noncrystalline or amorphous material – arrangement of atoms holds for a short range (glass)

Single crystal – consists of one large crystal (chip made from silicon)

Polycrystalline material – many small crystals with varying orientations (grains)

Liquid crystal: polymeric materials have a special type of order

- Behaves like amorphous material in one state (liquid-like).
- Some polymer molecules undergo crystalline structure in small zone with external electric field or temperature change
- Used in liquid crystal display (LCD) technology

Hard sphere model

Now we try to shift to the crystal structure of a specific material. So, crystal structure, the next level of the atomic structure where we can find out that the different atoms arranged want a specific sequence. When the regular (re) repetitive arrangement of atoms or ions actually exist over a long range which is typically more than hundred nano meter, then it forms a crystalline structure.

Non-crystalline structure, the difference is that arrangement of atoms holds for a short-range. Of course the long-range and short-range it is a scale specific, long-range we can consider which is (le) a length of the scale is above 100 nano meter and that is called, that actually forms the crystallline structure and (if) if the scale is less than the less than even typically less than 100 nano meter then it generally holds for short-range of noncrystalline solids. For example glass is a noncrystalline solid.

Now single crystal consists of one large crystal that is follow some specific arrangement of the atoms and poly crystalline material which is having so many crystal but with the, which having varying orientation and within that it forms one specific grains. Nowadays we also observed the liquid crystal as well but liquid crystal is the specific polymeric materials having a special type of order. And, but, it behaves like a amorphous material in one state specifically in the liquid state.

But some polymer molecules undergone crystalline structure in a small zone with some external electrical feed for temperature change. So this principle is applied in the liquid crystal display i. e. LCD technology. But when we try to analyse the crystal structure of a solid material we assume the shape of the atom as a spherical. So, that is called typically hard sphere model. So, based on the spherical structure of of an atom we try to analyse the crystal structure of specific material.

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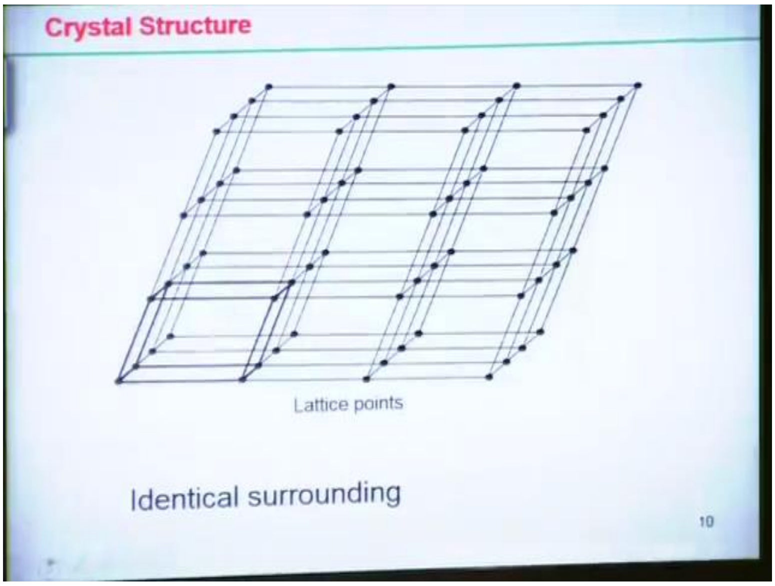

Crystal Structure

Identical surrounding

So it starts with the very basic things that is called the lattice. Lattice are the specified points in a three-dimensional (s) space where it follows some identical arrangement of the atoms and if we see that is point is considered as a lattice point.

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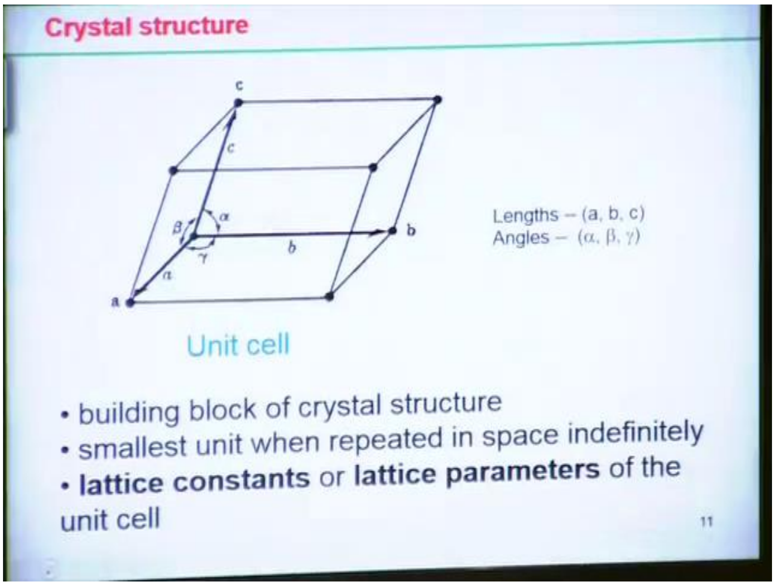

Crystal structure

Lengths – (a, b, c)
Angles – (α, β, γ)

Unit cell

- building block of crystal structure
- smallest unit when repeated in space indefinitely
- **lattice constants** or **lattice parameters** of the unit cell

So while we try to analyse the crystal structure of a specific material first step is to represent the structure in the form of unit cell. So unit cell is actually building block of the crystal structure and it represents the smallest unit where we can find out the characteristics of all the atomic (arrange) arrangements of a specific structure. But corresponding to each points, is can be defined as the lattice point and the parameters are called as the lattice parameters; for example if we see in the figure the length of the edge is defined a, b, and c and angles are the alpha, beta and gamma.

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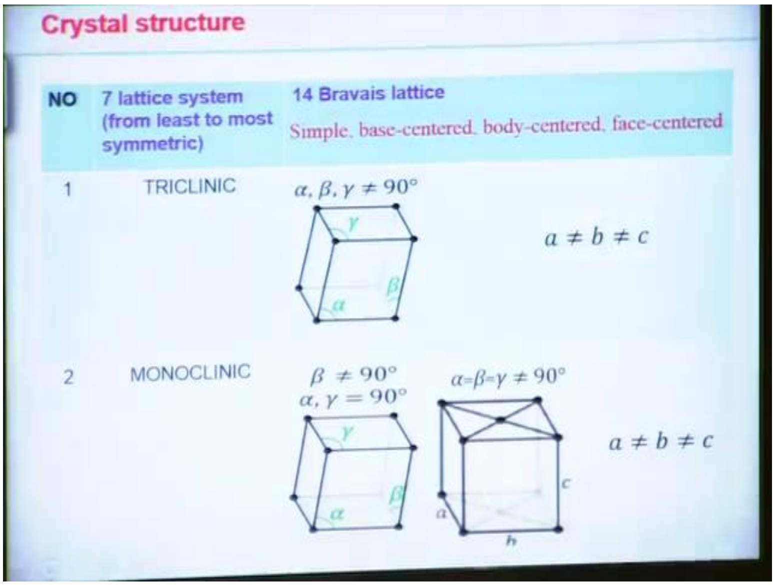

Crystal structure

NO	7 lattice system (from least to most symmetric)	14 Bravais lattice Simple, base-centered, body-centered, face-centered	
1	TRICLINIC	$\alpha, \beta, \gamma \neq 90°$	$a \neq b \neq c$
2	MONOCLINIC	$\beta \neq 90°$ $\alpha, \gamma = 90°$ $\alpha = \beta = \gamma \neq 90°$	$a \neq b \neq c$

Actually the 6 parameters constitute the different type of substructure of a specific material. So looking into these 6 parameters there are several variations of the atomic arrangement of the atoms. That we can categorise as 7 lattice system which actually says that from the least to the most symmetric part of the structure. And with the 4, 7 lattice system we can constitute the 14 numbers of Bravais lattice and this atoms can be arranged at a simple base centred, body centred and face centred positions.

Let us look into what are the different (base) 7 lattice systems and corresponding the type of the lattice structure. First is the triclinic. So, in triclinic structure, if we look into that here the dimensional is a, b and c they are not equal and alpha, beta and gamma, these are the not as 90 degree. And this is also (sim) this is, can be called as a simple structure.

Next if we look into that monoclinic structure. In the structure if we see here the simple structure as well as base centred structure. In simple structure, the one of the angle is not equal to 90 degree but other 2 angles are 90 degree. And here all the edge lengths are not equal with each other. In base centred structure if we look here, all the 3 angles are not equal and edge lengths are also not equal.

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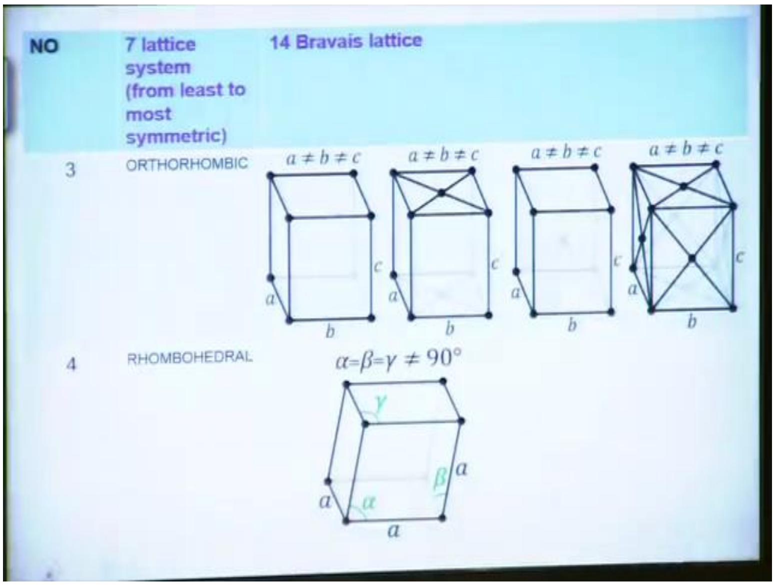

NO	7 lattice system (from least to most symmetric)	14 Bravais lattice			
3	ORTHORHOMBIC	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$	$a \neq b \neq c$
4	RHOMBOHEDRAL	$\alpha=\beta=\gamma \neq 90°$			

Now orthorhombic structure, in this case which is having 4 different types of structure; simple, base centred, body centred and face centred structure. So here the typical characteristic is that all the edge lengths are not equal but the angles alpha, beta and gamma all are 90 degree. So this constitute 4 different types of orthorhombic crystal structures. Now rhombohedral structure; you are all the angles are not equal but (edge) edges are equal and this constitute only the simple structure.

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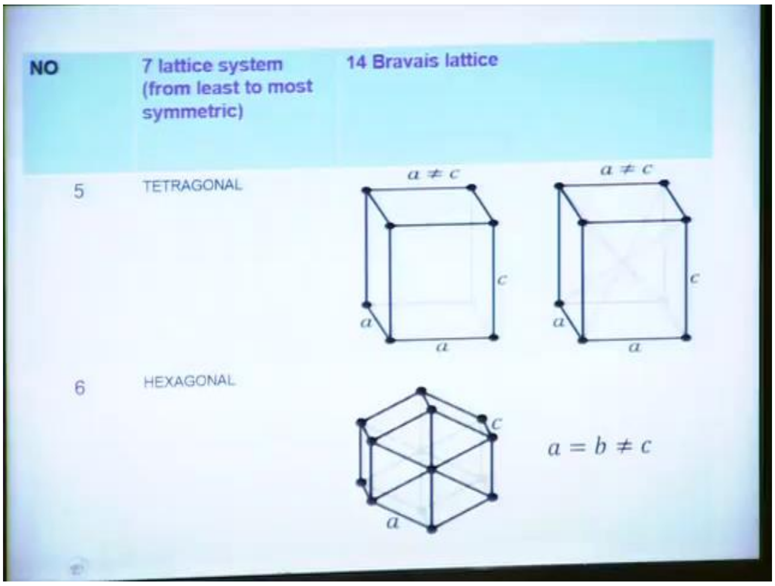

NO	7 lattice system (from least to most symmetric)	14 Bravais lattice
5	TETRAGONAL	
6	HEXAGONAL	$a = b \neq c$

Tetragonal structure is the, where 2 edges are equal but the not the third edges are not equal to others. And it constitute 2 different simple structure as well as body centred structure. Here the hexagonal structure, here (in) in this structure the 2 edges are equal but which is not equal to the height.

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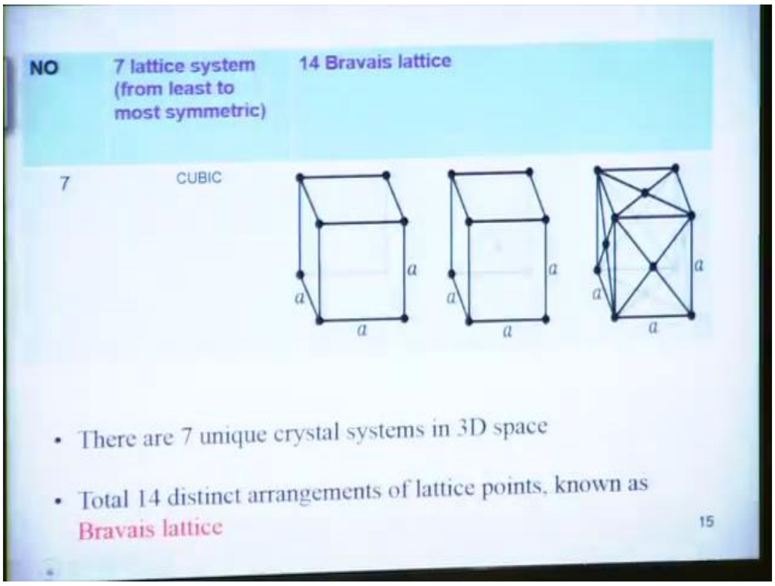

NO	7 lattice system (from least to most symmetric)	14 Bravais lattice
7	CUBIC	

- There are 7 unique crystal systems in 3D space
- Total 14 distinct arrangements of lattice points, known as Bravais lattice

In cubic structure we found out that simple structure, body centred structure and faces centred structure; here all the angles are equal to 90 degree as well, all the edges are equal. So in summary we can say there are 7 unique crystal structure in 3-dimensional space and there are 14 distinct arrangement of the lattice points which is known as the Bravais lattice. So based on this crystal structure we can analyse further, for different type of engineering materials which used in common, in the commonly.

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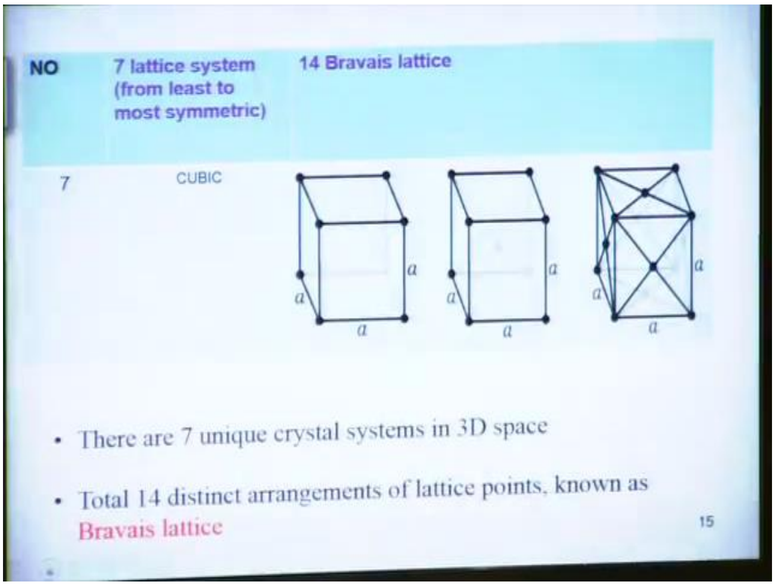

NO	7 lattice system (from least to most symmetric)	14 Bravais lattice
7	CUBIC	

- There are 7 unique crystal systems in 3D space
- Total 14 distinct arrangements of lattice points, known as Bravais lattice

Crystal structure of a specific material can be based on the lattice and the basis. Lattice is simply a point in a 3-dimensional space and basis is corresponding to a group of single bond atom or a group of atoms that is located on (s) specific sequence or in a particular way and also associated with the lattice point. So crystal structure actually combine effect of the both lattice point as well as basis. Normally in case of the pure metal one single lattice point there exists single atom and if a compound materials one single lattice point there may be a, there may exist the, more than 1 atoms (on) on that specific lattice point. This is the (basic) very basic structure of a crystal.

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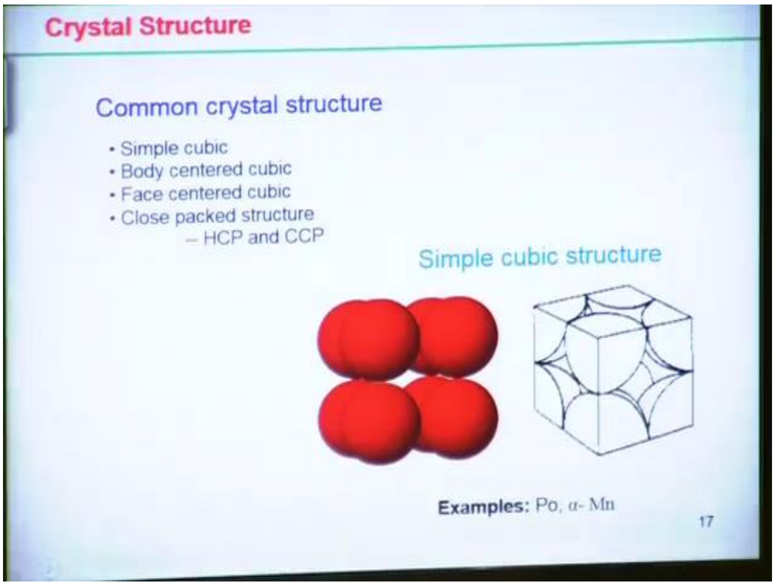

Crystal Structure

Common crystal structure

- Simple cubic
- Body centered cubic
- Face centered cubic
- Close packed structure
  - HCP and CCP

Simple cubic structure

Examples: Po, α- Mn

Now we will try to analyse the very common crystal structure; first is the simple cubic structure. In simple cubic structure the figure shows that the arrangement of the atoms on a cube at 8 different corners. So, that 8 different corners and there is a space also inside the centroid of the crystal. In this case the Polonium actually follow this type of crystal structure, but it is to be noticed that the induced cell consists of a part of the atoms not the full volume of the atoms exist within the unit cell.

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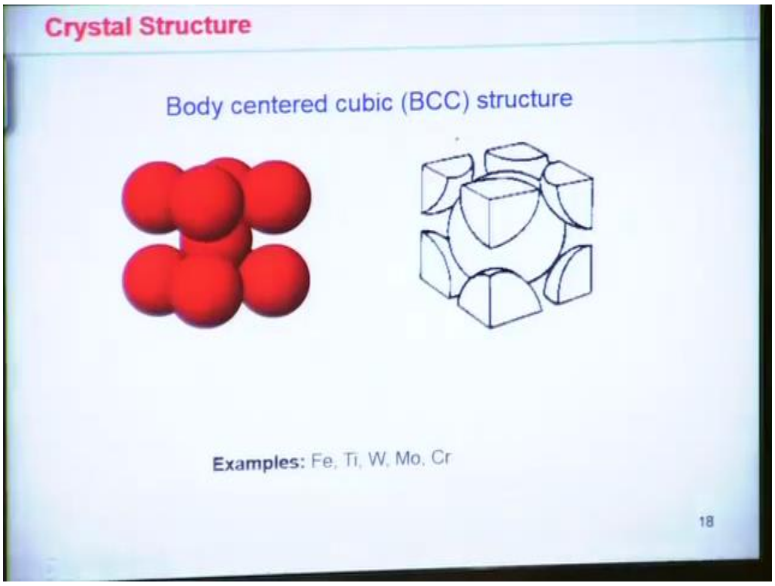

Crystal Structure

Body centered cubic (BCC) structure

Examples: Fe, Ti, W, Mo, Cr

(So) so now we look into the body centred cubic structure that is called the BCC structure. in BCC structure there exist 8 atoms at the corner, at the same time 1 atoms exist at the centroid of the cube within the body (i) within the body itself. So in this case the iron, titanium, tungsten, molybdenum, chromium; they actually follow this type of structure.

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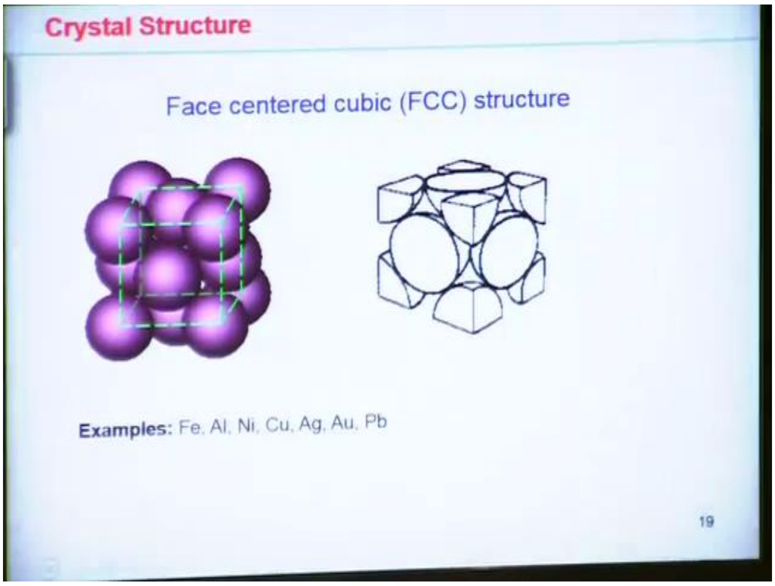

Crystal Structure

Face centered cubic (FCC) structure

Examples: Fe, Al, Ni, Cu, Ag, Au, Pb

Face centred structure, that is called FCC structure, apart from the 8 cornered atoms there are 6 spaces, on the 6 spaces there exists 6 (diff) atoms also. Iron, aluminium, nickel, copper, silver; these type of materials actually follow the FCC structure. So it is to be noticed that the iron also having BCC structure as well as FCC structure also. So, that we will discuss later on.

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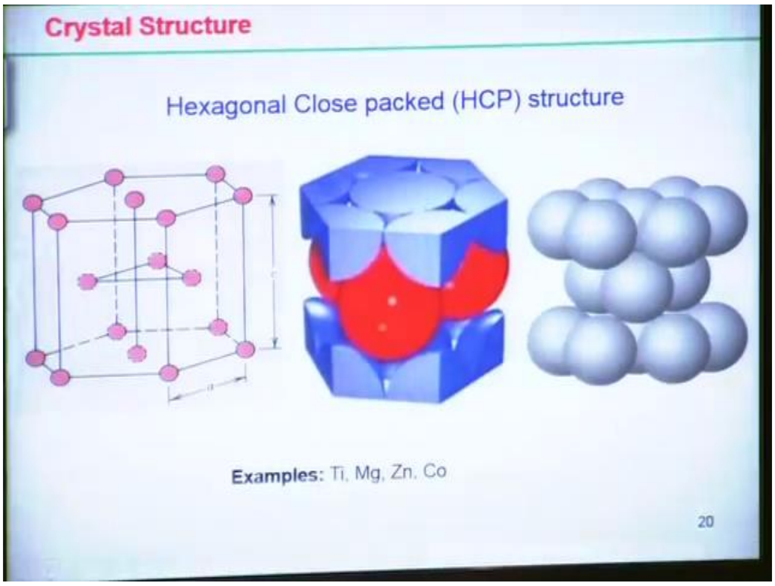

Crystal Structure

Hexagonal Close packed (HCP) structure

Examples: Ti, Mg, Zn, Co

20

This is one of the most common structure that is called hexagonal close packed structure, (I) HCP structure; here you can see that the that on the face there are 6 atoms exist and the inside the atoms, inside the structure itself there exist the metal layer, 3 atoms again the repetition of the same arrangement on the top surface. So this is the constitution of the hexagonal close packed structure and titanium, cobalt, zinc actually follow this type of structure.

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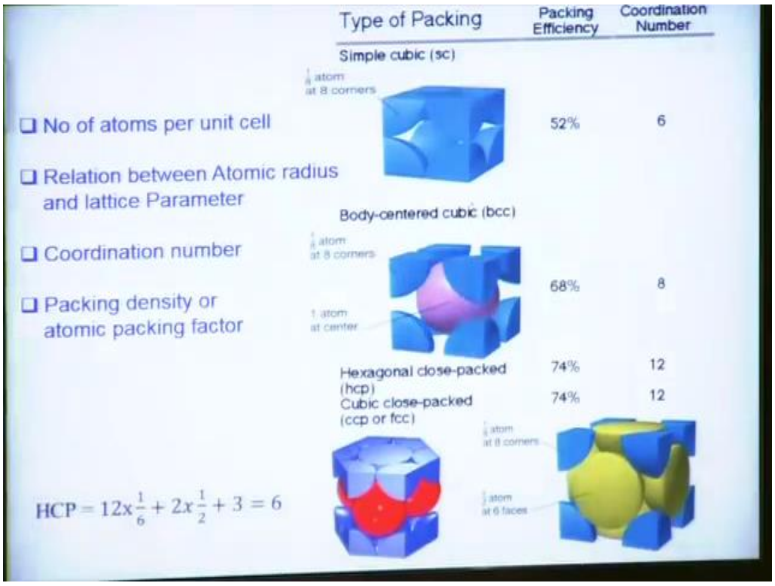

- ☐ No of atoms per unit cell
- ☐ Relation between Atomic radius and lattice Parameter
- ☐ Coordination number
- ☐ Packing density or atomic packing factor

Type of Packing	Packing Efficiency	Coordination Number
Simple cubic (sc)	52%	6
Body-centered cubic (bcc)	68%	8
Hexagonal close-packed (hcp)	74%	12
Cubic close-packed (ccp or fcc)	74%	12

$$HCP = 12x\frac{1}{6} + 2x\frac{1}{2} + 3 = 6$$

So apart, now if we look into the typical parameters when we try to explain the different common crystal structure like simple cubic BCC structure, FCC structure and HCP structure. So here it is mandatory to know that what is the total number of (ex) atoms associated within the unit cell of this different type of crystal structure. What are the relation between the atomic radius and the lattice parameter? How we can estimate the coordination number and and what are the coordination number for all these 4 basic type of crystal structure and what are the packing density or (am) atomic packing factor for this type of crystal structure?

So first if we look into the simple (cube) cubic structure, here we see that there exist only 8 cornered atoms and sharing of the atoms is 1 eighth volume within the unit cell. So 1 eighth into 8 that actually represents the only 1 number of atoms exist within the unit cell of the simple cubic structure. Now we look into the coordination number. What is the coordination number? So if we pick up any of the atoms within the unit cell, and if you try to find out the continuity of the atoms which in continuous contact with the surrounding atoms then we can find out the coordination number of a specific atom.

So in this case if we consider anyone of the atom of the simple cubic structure and if we look 3 different direction, may be X, Y and Z we will be able to find out, there is a continuous contact in X direction, 1 atom with another 2 atoms, in Y another 2, in Z another 2. So, here the coordination number is 3 into 2 that is 6. Now packing fraction; packing fraction actually decides the what is the amount or what is the volume of the atoms occupied within the unit cell. So it is the typically the ratio of the volume of the atoms within the unit cell and the total volume of the unit cell.

So in this case it is also necessary to know the relation between the lattice parameter and atomic radius of the atoms. So in this case since we need to know the contact between the atoms, so in simple cubic structure along the (edge) edge 2 atoms are in contact. So if the lattice parameter is A then we can write A equal to 2 into R where R is the atomic radius. So this is the relation between the lattice parameter A and the atomic radius.

So now if we look into that BCC structure and if we try to find out what is the coordination number and what is the total number of atoms in BCC unit cell. Here if you see that there are 8 cornered atoms and 1 body atom. So 8 cornered atoms actually share the 1 eighth of the volume and the body centred atoms fully exist within the unit cell. So then, here total number of atoms equal to 2 in this case. Now if we look into that coordination number in this case if we consider the body centred atoms so it is very clearly associated with the 8 cornered atoms so that the coordination number is 8 in this case.

But, what may be the relation between the lattice parameter and the atomic radius in this case? So, we need to know the atomic arrangement of this specific crystal structure then we can easily find out this co-relation. Let us look into the structure. Here the atoms, cornered atoms is not are in continuous contact between the, along the edges. In other words, it is in continuous contact along the body diagonal. So, looking into that the body diagonal, if the lattice parameter is A, so body diagonal actually represents root 3 A.

So that is kind of continuous contact is like that; so in this case we can say that root 3 A equal to R plus twice R plus R. So that is 4R. So this is the relation between the lattice parameter and the atomic radius. So this can be easily derived if the arrangement of the atoms is known already for a specific crystal structure. Now packing factor in this case we can easily find out, what is the volume of their atoms within the unit cell divided by the volume of the, total volume of the unit cell. In that way we can find out the packing fraction is 68 percent in this case.

Now if we look into the cubic close packed structure or (BC) FCC structure then we can find out the number of atoms associated with these unit cell, there exist 8 cornered atoms having 1 eighth sharing and there also exist the 6 face atoms but sharing is only 50 percent within the unit cell. So in this case total number of atoms 1 eighth into 8 cornered atoms and half sharing for 6 faces. So, that means total number of atoms is 4 in FCC crystal structure.

Now in similar way we can find out the number of atoms in case of HCP crystal structure. Here you can see there are 12 atoms on the bottom face and of the upper side so total 12 atoms, but sharing each only 1 sixth volume of the atoms and 2 face atoms which is sharing is the 50 percent and there are the 3 atoms which exist inside the volume of the hexagon. So in this case total number of atoms in case of HCP structure is 6.

So now if we observe that the packing efficiency for the FCC structure and the HCP structure is 74 percent, so among all these materials this is the having the highest packing efficiency. That means the atoms are most densely packed in case of FCC (st) HCP structure as compared to the BCC structure and simple cubic structure. So this all the analysis can be useful for the, to solve any kind of other different type of problems.

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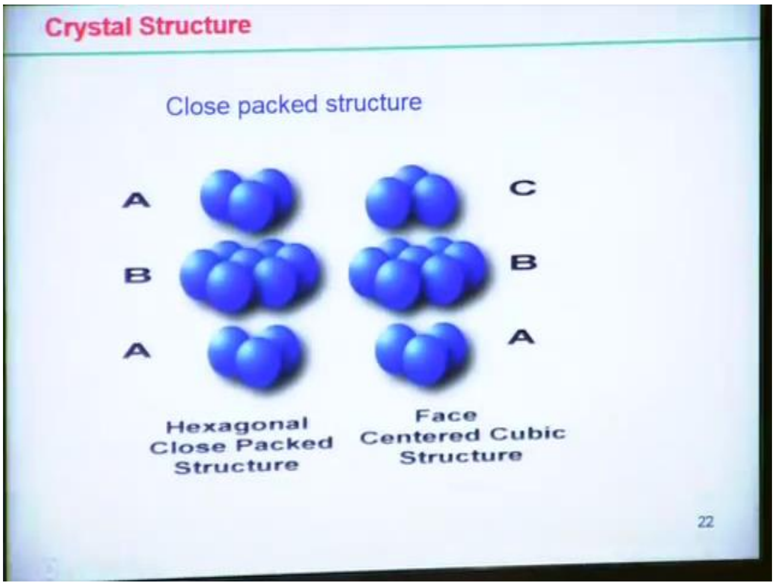

Crystal Structure

Close packed structure

Now of course when we try to represent the different type of common structure using the different, representing the different unit cell we can find out that actually this is, this follows some specific sequence of the atoms. For example, in hexagonal close packed the one layer, if we assume this is as the layer A, arrangement of the atoms; next layer is the B and next layer as the A, again next layer as a B; so there is alternate arrangement of the atoms we generally observe in the hexagonal close packed structure.

But in case of FCC structure it is the atomic arrangement also not the alternate sequence of different layer for maybe we can say this is a different stacking sequence. Here the stacking sequence actually follow in this way the A wants specific arrangement of the atoms, second layer which is the B, it is (())(46:47); then third layer it is C, again the repetition of the same

A, B, C. So, basically the atomic arrangement in FCC structure follows 3 different A, B, C layers, but it is not the case of the HCP structure, HCP structure it follows in that way A, B, A, B in that sequence. Of course when you try to say the FCC structure follow A, B, C in this sequence, but that sequence follow normal to a specific plane in case of FCC structure that we will discuss later on.

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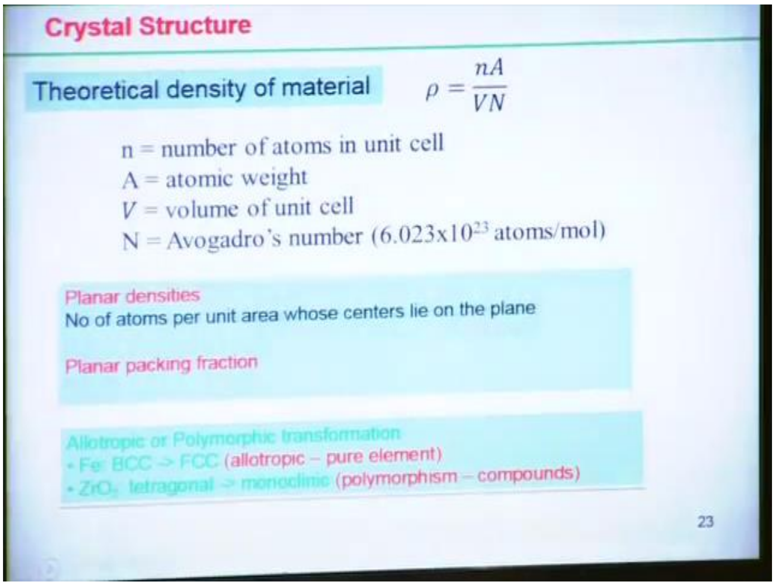

Crystal Structure

Theoretical density of material $\rho = \frac{nA}{VN}$

n = number of atoms in unit cell
A = atomic weight
V = volume of unit cell
N = Avogadro's number ($6.023\text{x}10^{23}$ atoms/mol)

Planar densities
No of atoms per unit area whose centers lie on the plane

Planar packing fraction

Allotropic or Polymorphic transformation
- Fe: BCC -> FCC (allotropic – pure element)
- ZrO_2: tetragonal -> monoclinic (polymorphism – compounds)

Now looking into the different type of (pures) crystal structure what is the, for different material it is possible to know the estimate, the theoretical density of the material. So, specifically the density can be defined as the ratio of the mass and volume. So, in this case we can find out rho equal to nA by V into N where A is the number of atoms in a unit cell, that we can easily estimate, second is the atomic weight of a specific material that is (())(48:10), and third is the volume of the unit cell; if we know the lattice parameter or if we know the relation between the atomic radius and the lattice parameter for (s) for a specific material then we can find out the volume of the unit cell and N is the typically Avogadro's number. So by the using this formula we can find out the theoretical density of a specific material. So, of course it can be used also compound material but so far we have discussed the crystal structure of the different materials but that is in case of the pure metal.

Now other mathematical calculation can also be done by looking into the crystal structure that is called planner densities; sometimes it is important to know this parameter, planar packing fraction also. So, planar packing fraction is the, what are the fraction occupied by the atoms over a plane, not the over entire volume of the unit cell. Similarly, planar density can be defined, what is the total number of atoms for unit area, so, on a specified plane only.

So if we know all this parameter then we can easily find out planar density and planar packing fraction of a specific material. So what, there is a difference between the planar density and planar packing fraction. Planar density actually represents the number of atoms per unit area but planar packing fraction is a simply the ratio or some numericals.

Now to important things are there, as I mentioned that iron can exist 2 different type of crystal structure depending upon the different temperature range like so that type of transformation is called the allotropic transformation and this allotropic (trans) transformation is generally used for the, this term is generally used for the pure element.

For example, iron can be transferred from BCC structure to FCC structure. So in this case it is associated with some volumetric change. So this needs to be addressed when you try to analyse that allotropic transformation of pure metal and of course it happens within over a specific range of temperature.

Next is the polymorphism or polymorphic transformation, so polymorphic transformation is associated with the compound material; for (exa) example germanium oxide, where it transforms from tetragonal to monoclinic structure. Of course it is associated with some volumetric change.

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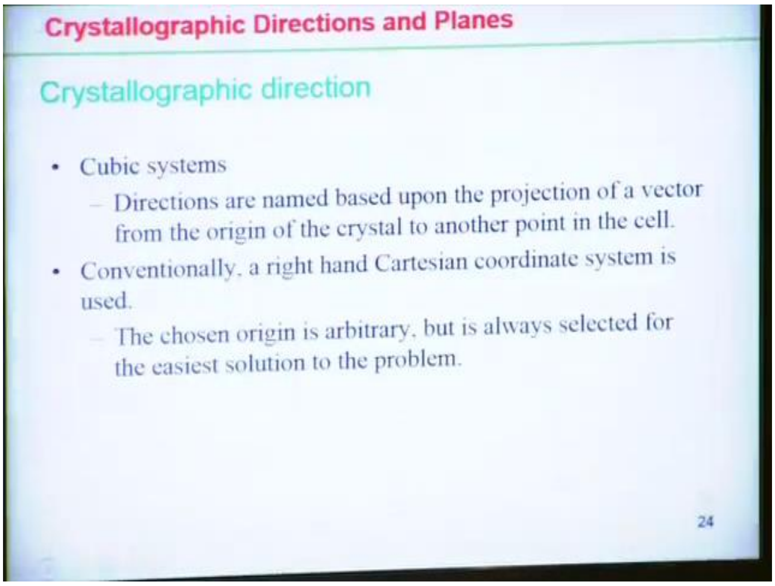

Crystallographic Directions and Planes

Crystallographic direction

- Cubic systems
  - Directions are named based upon the projection of a vector from the origin of the crystal to another point in the cell.
- Conventionally, a right hand Cartesian coordinate system is used.
  - The chosen origin is arbitrary, but is always selected for the easiest solution to the problem.

Now this is a basic crystal structure of a very simple materials (of) specifically for the pure metals we have analysed; now we will try to focus on the crystallographic direction and crystallographic planes and how we can decide the crystallographic direction. So, we will try to focus on first the cubic system. In this case direction can be find out upon the projection of a vector after choosing the origin of a specific crystal structure of fixing the different axes. Conventionally a right-hand coordinate system is generally followed but the origin can be chosen arbitrarily, but we choose all this case to look into the interest of the easiest solution of the problem.

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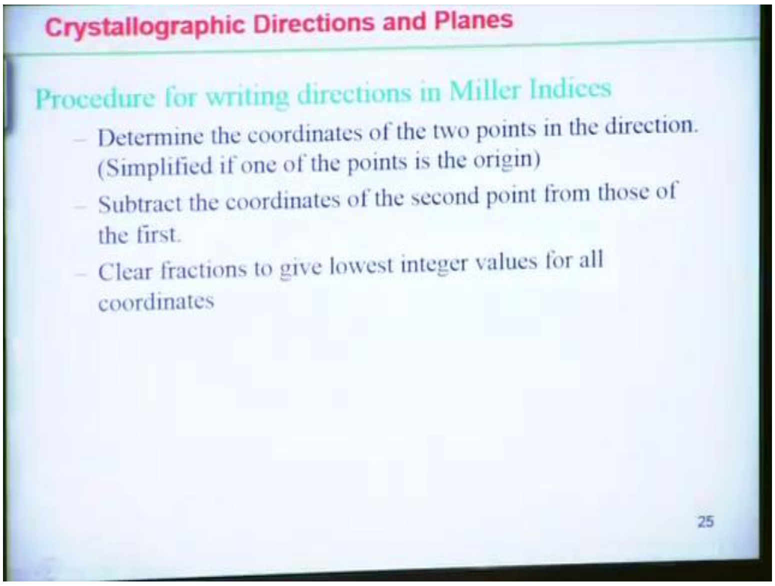

Crystallographic Directions and Planes

Procedure for writing directions in Miller Indices

- Determine the coordinates of the two points in the direction. (Simplified if one of the points is the origin)
- Subtract the coordinates of the second point from those of the first.
- Clear fractions to give lowest integer values for all coordinates

Let us look into the example then it may be very much understood. Procedure for the writing directions in Miller Indices; specifically when you try to represents the direction in a specific crystal structure that is called the Miller Indices and we represent in terms of the Miller index in this case. First we try to determine the coordinates of the 2 different points and then subtract the coordinates of the second point from those of the first, and then clear the fraction to give the lowest integer values for all the coordinates and we represents this as a direction in case of specific crystal.

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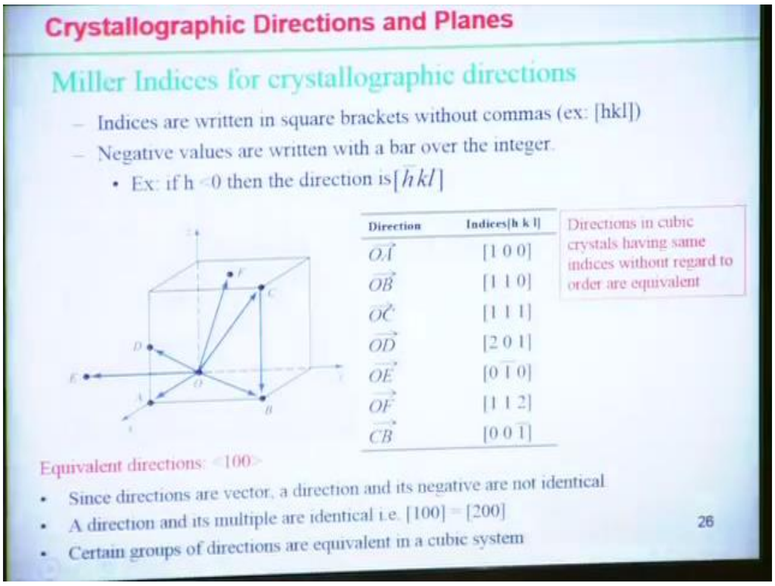

Crystallographic Directions and Planes

Miller Indices for crystallographic directions

- Indices are written in square brackets without commas (ex: [hkl])
- Negative values are written with a bar over the integer.
  - Ex: if h < 0 then the direction is $[\bar{h}kl]$

Direction	Indices[h k l]
$\overrightarrow{OA}$	[1 0 0]
$\overrightarrow{OB}$	[1 1 0]
$\overrightarrow{OC}$	[1 1 1]
$\overrightarrow{OD}$	[2 0 1]
$\overrightarrow{OE}$	$[0\ \bar{1}\ 0]$
$\overrightarrow{OF}$	[1 1 2]
$\overrightarrow{CB}$	$[0\ 0\ \bar{1}]$

Directions in cubic crystals having same indices without regard to order are equivalent

Equivalent directions: <100>

- Since directions are vector, a direction and its negative are not identical
- A direction and its multiple are identical i.e. [100] = [200]
- Certain groups of directions are equivalent in a cubic system

Let us look into the several examples for the Miller Indices of the crystallographic directions. First, first point is that index are written in the square bracket but without commas, that example is given like this, the square bracket and hkl in this form. Next point is that negative values are written within a bar over the integer, but, for example if h less than 0 that means if it is negative then the direction can be represent is like this.

If we look into that figure, so first to find out the Miller index of a specific crystallographic direction we need to choose the origin. Suppose this point is chosen as origin and then following the right-handed coordinate system we choose the axis X, axis Y and axis Z. Now let us look into how we represents the direction OA, if we look into that, direction OA is corresponding to this 1 0 0. So it is like that the coordinate of A is 1 0 0 and final coordinate of the origin simply 0 0 0. So resultant is the 1 0 0. But when you try to represent in terms of Miller index we represents in the third pattern. So h first component, K 0, L 0, like that. So 1 0 0 actually represents the X as (on) OA within the unit cell (while) when we have specified the origin and the 3 different axes.

Now how we can represent OB; if you look into that OB, OB, so here if you look into that OB, OB can be represented like that 1 1 0. So coordinate of B is specifically that X component is the 1, Y component is 1and Z component is 0. So accordingly we can find out the direction OB is 1 1 0.

Let us look into the direction OE. Assuming that OE along the Y direction it is of unit length. So in this case the X component is 0, Y component is negative direction of Y, so minus 1 and

Z component is 0. Now coordinate of origin 0 0 0; so finally OE represents 0 minus 1 0. So when you try to represents in terms of the Miller index then it will be third bracket 0 1 0 but negative integer value can be represents over a bar like this. So this is the Miller index of the direction OE. So similarly we can find out the different directions OA CB in the similar fashion.

Now equivalent direction; so since directions are vectors so direction and its negative are not identical. Same time direction and its multiple are identical, specifically 1 0 0 or 2 0 0 indicates the similar direction. Certain group of direction are equivalent in a cubic system if we change the axis coordinate or if we exchange if we transform the axis X Y Z, so it represents probably the similar direction can be present at the form of as a group, like that group can be written in this point. For example, 1 0 0 in the group, it actually represents the axis X, along X, along Y as well as along Z also. So this is a bulk can be represents in the equivalent form or as a family form or as a group.

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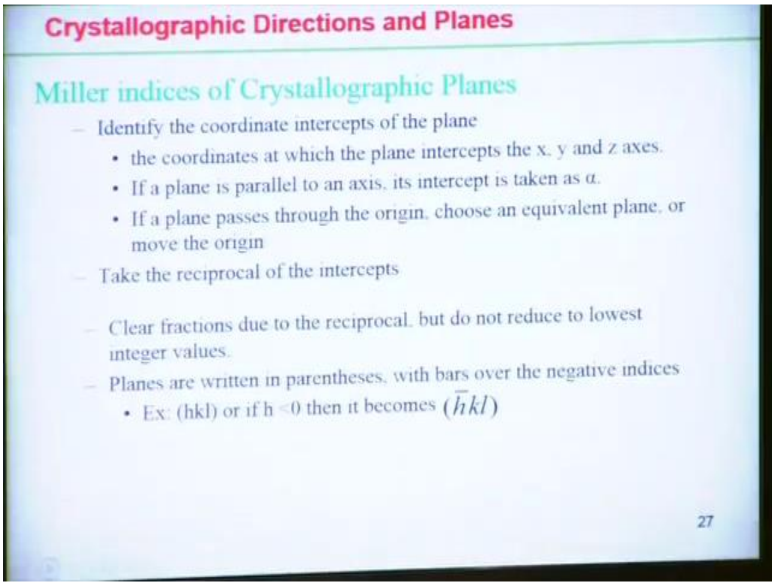

Crystallographic Directions and Planes

Miller indices of Crystallographic Planes

- Identify the coordinate intercepts of the plane
  - the coordinates at which the plane intercepts the x, y and z axes.
  - If a plane is parallel to an axis, its intercept is taken as α.
  - If a plane passes through the origin, choose an equivalent plane, or move the origin
- Take the reciprocal of the intercepts
- Clear fractions due to the reciprocal, but do not reduce to lowest integer values.
- Planes are written in parentheses, with bars over the negative indices
  - Ex: (hkl) or if h <0 then it becomes $(\bar{h}kl)$

Now we can represents the crystallographic plane in terms of the Miller index form. But in this case we need to first identify the coordinate that intersects on, intercepts on the different axis. The coordinates at which the plain intercepts along the X Y and Z axis need to find out first. If the plane is parallel to an axis then it intercept can be considered as Infinity, if the plane passes through the origin then in this case we can shift the origin or we can consider other equivalent plane.

Next step is to find the reciprocals of the intercepts; next clear fractions to the reciprocals but not necessary to reduce the lowest integer values. Planes are written in parentheses were the bars indicates the negative index; for example if h less than 0 then it can be represents the plane in terms of this which is different from the directions where we use generally the square bracket. Let us look into some example to find out the Miller index of a specific plane.

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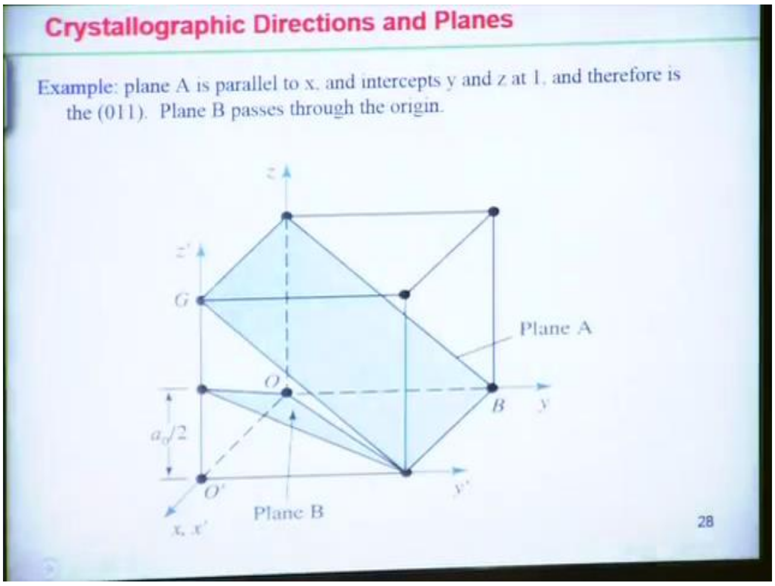

Crystallographic Directions and Planes

Example: plane A is parallel to x, and intercepts y and z at 1, and therefore is the (011). Plane B passes through the origin.

Example; the plane A if we look into the figure which (is) the plane A is parallel to the x; so parallel to the x-axis that may intercept with respect to x-axis can be considered as Infinity, but the intercepts along Y and Z 1 and Z also 1. Now next step is to take the reciprocals of all this intercept length; represents clear the fraction, 0 becomes 0 1 1. So the Miller index of this plane is 0 1 1. Now if we look into the plane actually B; the plane B actually passes through the origin so in this case we need to shift the origin or we need to consider all the equivalent plane and then we can find out the Miller index of this plane.

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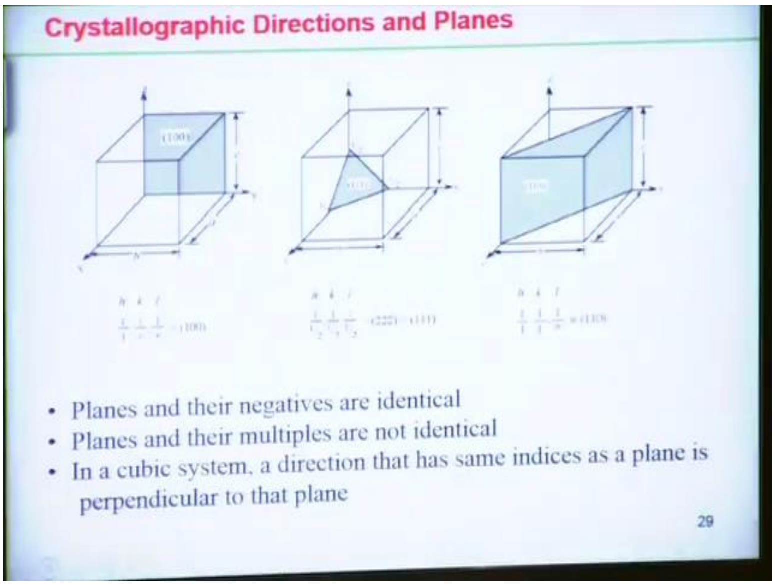

Crystallographic Directions and Planes

- Planes and their negatives are identical
- Planes and their multiples are not identical
- In a cubic system, a direction that has same indices as a plane is perpendicular to that plane

Let us look into several examples so it may be more, it will be more obvious to find the Miller index of the different planes. Let us look into the first figure; in this case we have defined the origin and we have defined the 3 different axis. So the highlighted plane 1 0 0 it is actually represents basically Y Z plane. And so intercept along X Y and Z can be considered as a unit length along the X it can be unit length. So along Y the intercept length it is parallel to the Y axis so intercept length can be Infinity.

Z also the; it is parallel to the Z axis at the same times the intercept can be considered as Infinity so finally the Miller index will be the 1 0 0.But here we observe that this plane actually passes through the origin, but in this case we can shift the origin to some other point and then accordingly we can constitute the X Y and Z axis then we can decide the Miller index of this specific plane.

Second figure if we look into that the highlighted plane here the 1 1 1 plane so that plane actually intercepts the X Y and Z axis in the half, half and half; so if we take the reciprocals of half, half, half and then we can find out 2 2 2 but we can reduce the integer and it is can be written as 1 1 1. So, this indicates the specifically 1 1 1 plane, okay? And of course the 1 1 1, 2 2 2 or maybe 3 3 3, that actually represents the different parallel planes.

So third one we look that, that this plane actually it is the, first it is parallel to the Z axis so intercept length is Infinity, Z axis, but it intercept length along, X and Y both are 1. So if we take the reciprocal then it becomes 1 by 1 and 1 by Infinity, so finally it becomes 1 1 0. So this is the this is the plane. So these are the typical ways to find, estimate the different planes (in) and find out the Miller index of a specific plane in a crystallographic structure. But it is to be noticed that planes and their negatives are identical but planes and their multiples are not identical but in a cubic system, a direction that is same index is a plane is perpendicular to the, to that plane. This is a very significant conclusion that to be useful for the further calculation.

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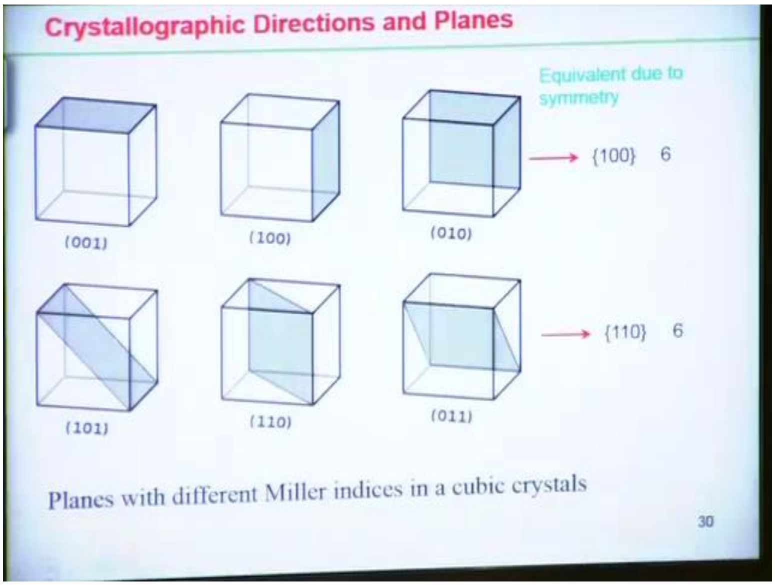

Crystallographic Directions and Planes

Equivalent due to symmetry

{100} 6

{110} 6

Planes with different Miller indices in a cubic crystals

Let us look into the other examples, the different planes 0 (1) 0 0 1, 1 0 0, 0 1 0, and actually this different planes which can be form in the equivalent form and this is equivalent due to the symmetry and there exists such 3 different planes simply the changing of the position of 1. So maybe 1 0 0, 0 1 0, 0 0 1 and their negative values can constitute 6 different types of the planes and in the equivalent form it can be written as the second bracket in this form. Similarly the 101 frame while changing the position of 1 1 0 we can represents the different planes in the 6 different ways and all actually represents the in the equivalent form.

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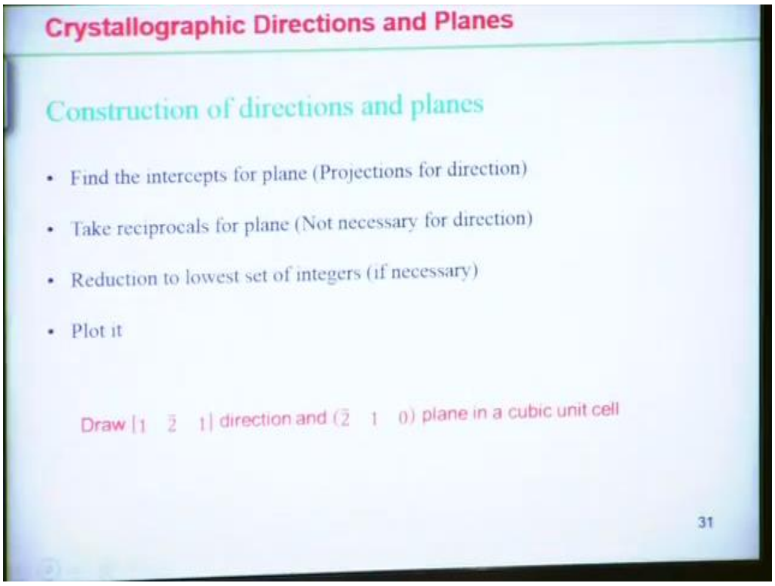

Crystallographic Directions and Planes

Construction of directions and planes

- Find the intercepts for plane (Projections for direction)
- Take reciprocals for plane (Not necessary for direction)
- Reduction to lowest set of integers (if necessary)
- Plot it

Draw $[1\ \bar{2}\ 1]$ direction and $(\bar{2}\ 1\ 0)$ plane in a cubic unit cell

Apart from the identification of the Miller index of a specific plane within the unit crystal structure it is also necessary to know how to construct the different direction in planes in a unit cell. First it is necessary to know what is the intercepts of a specific plane and then (consider) consider the reciprocals of that plane but not necessary for the direction and try to reduce the lowest set of integer in this case. And, then we can finally plot it. So drawing the different type of planes in a (cu) cubic unit cell may be useful so this can be considered later on as an assignment how to draw the different type of planes and directions in a unit cell.

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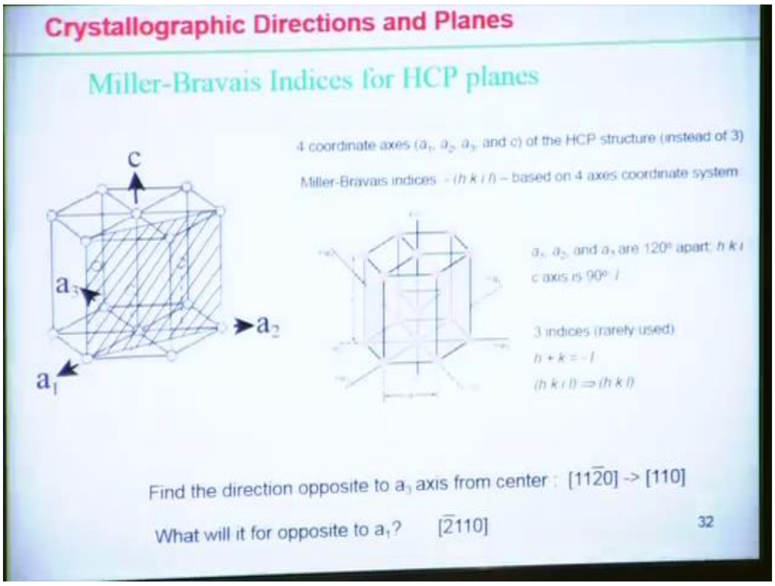

Crystallographic Directions and Planes

Miller-Bravais Indices for HCP planes

4 coordinate axes (a_1, a_2, a_3 and c) of the HCP structure (instead of 3)

Miller-Bravais indices - ($h\ k\ i\ l$) – based on 4 axes coordinate system

a_1, a_2 and a_3 are 120° apart: $h\ k\ i$

c axis is 90°: l

3 indices (rarely used)

$h + k = -i$

$(h\ k\ i\ l) \Rightarrow (h\ k\ l)$

Find the direction opposite to a_3 axis from center : $[11\bar{2}0] \rightarrow [110]$

What will it for opposite to a_1? $[\bar{2}110]$

Now in case of (hexta) hexagonal close packed structure we try to represents directions on planes but here the difference from the cubic structure is that cubic structure we represents there is a 3 components or basically 3 axis system. But, in this case we need to define the 4 coordinate axis. 1 is the a1, a2 and a3; its lie 1 specific plane and another is the height c. this is a typical arrangement for the HCP structure and this type of index is called Miller-Bravais Indices for (hexta) hexagonal close packed structure.

So here if we see that there is a co-relation between the 3 axis system and the 4 axis system, that is the hexagonal close packed structure to the cubic system. So I think it is not that scope of this (())(68:17) but that exists actually. Now we try to find out the direction opposite to the a3 axis from the Centre in a 4 axis system. So specifically what is the direction and how we can represent in terms of Miller (repre) index Indices in case of HCP structure. If we look into that and if we see that we need to define (f) first the coordinates of this point on the 3 axis system. So this axis, 3 axis system in hexagonal close packed structure actually exist the difference of 120 degree.

So opposite to the a3 axis actually the coordinate if we project on the 2 different axis, here if we consider as a total unit of length 2a along the axis; so this length actually represents the unit a, this length actually represents the unit a and a1, a along the a2 it is a but along the a3 it is minus twice a and, and the Z the coordinate is 0. So when you try to represents this in terms of the Miller Indices in the 4 axis system that is 1 1 2 bar 0. And that can be, using the co-relation that can be converted to the equivalent direction in case of 3 axis system or cubic system. So similarly, similar fashion we can construct the different direction maybe opposite to a1. So, rearrangement of this numbers which is corresponding to, opposite to a; similarly opposite to a2 we can find out; that can be, this represents actually opposite to a2.

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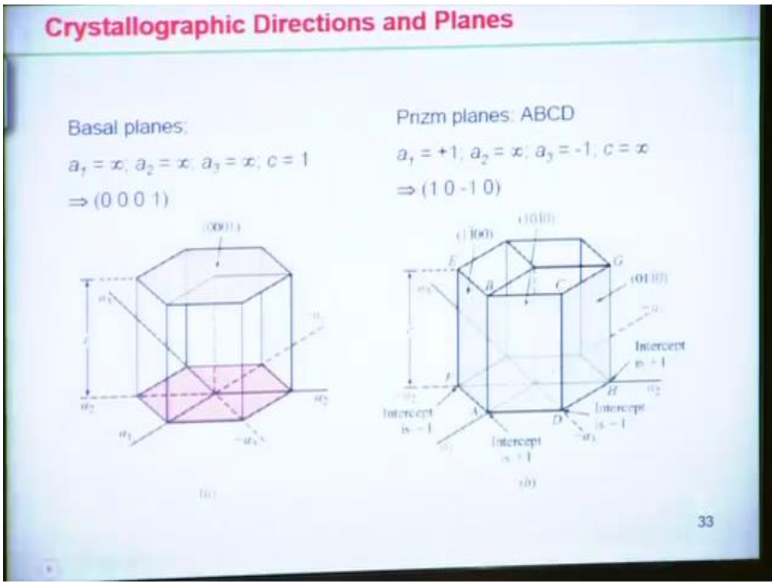

Crystallographic Directions and Planes

Basal planes:

$a_1 = \infty;\ a_2 = \infty;\ a_3 = \infty;\ c = 1$

$\Rightarrow (0\ 0\ 0\ 1)$

Prizm planes: ABCD

$a_1 = +1;\ a_2 = \infty;\ a_3 = -1;\ c = \infty$

$\Rightarrow (1\ 0\ -1\ 0)$

Similar way we can find out, we can define the different planes in case of HCP structure. Let us look into the some basal planes, maybe this plane. So here the; this plane is actually parallel to the, all the 3 axis a1, a2 and a3 but perpendicular to the, the intercept along the Z axis is unit 1. So, Infinity Infinity 1, if we took the reciprocals the planes can be represents as 0 0 0 1.

Similarly if we look into the other planes also for example the prism planes ABCD, this plane and before defining this plane first we fixed the axis a1, this is axis a2, this is axis a3 and this is axis c. So, in this case if we find out the (int) this plane intercepting another a1 axis, this is 1, along a2 axis it is parallel, along a2 axis it is parallel, so intercept length can be considered as Infinity. And along a3 it is intercepting a3 axis but in negative direction.

So that is considered as minus 1, at the same time this plane is parallel to the c axis. So the intercept length can be considered as Infinity. So in this case if you take the reciprocals, all these things, the plane can be represents as 1 0 minus 1 0 or 101 bar 0. So this is the typical representation of the specific plane in case of hexagonal close packed structure.

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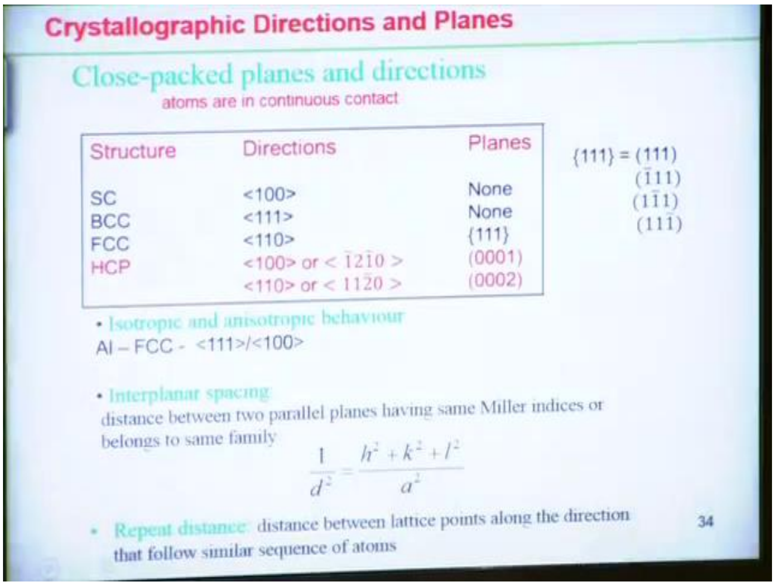

Crystallographic Directions and Planes

Close-packed planes and directions

atoms are in continuous contact

Structure	Directions	Planes
SC	<100>	None
BCC	<111>	None
FCC	<110>	{111}
HCP	<100> or $\langle \bar{1}2\bar{1}0 \rangle$ <110> or $\langle 11\bar{2}0 \rangle$	(0001) (0002)

$$\{111\} = (111),\ (\bar{1}11),\ (1\bar{1}1),\ (11\bar{1})$$

- Isotropic and anisotropic behaviour

Al – FCC - <111>/<100>

- Interplanar spacing

distance between two parallel planes having same Miller indices or belongs to same family

$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

- Repeat distance: distance between lattice points along the direction that follow similar sequence of atoms

Now, if we look into in the summary that different close packed planes and directions exist in the different type of crystal structure (ob) obviously we have discussed only the simple cubic BCC, FCC and HCP structures. So, among this simple cubic structure, the, we can observe the different close packed planes and different close packed directions. For example; simple cubic structure 1 0 0. So that is the along the edge of a crystal structure that is the close packed direction.

In case of BCC structure 1 1 1, so that means along the body centred, body diagonal that is the close packed structure in case of BCC, in case of FCC 1 1 0, that means it is the, along the face diagonal, this is the close packed structure and HCP, (also) having 1 2 1 0 or 1 1 2 0 these 2 types of close packed directions. So that means close packed directions that atoms are in continuous contact. Now if we find the, what are the close packed plane for this type of simple cubic (str) simple cubic structure and hexagonal structure we found the simple cubic and BCC structure not having any close packed planes because not any plane the all atoms are in continuous contact; but in case of FCC the close packed plane is 1 1 1.

So basically that 1 1 plane all the atoms exist in such a way, they are in continuous contact with each other, so that is why this game is considered as a close packed plane. In case of HCP structure as well we can find out the 0 0 1 or 0 0 0 2; these are the basically the parallel planes, so these are the either base plane; this represent the base planes, so that base planes all the atoms are in continuous contact; so that planes can be considered as a close packed planes.

Now this is all about the different type of structure, their directions. Now sometimes it is important to note the very specific elementary thing for example isotropic and anisotropic behaviour which very useful when we try to analyse the anisotropic behaviour in case of elasticity and (plastic) plasticity of a specific crystal structure. So aluminium, although it is FCC structure, but the material, their, arrangement of the atoms may not be the same in 1 1 1 or 1 0 0 direction. So that actually brings some anisotropic behaviour.

Interplanar spacing is the another elementary thing which is related to the crystal structure; that distance between 2 parallel planes having the same Miller Indices or belongs to the same family. So d is the interplanar spacing , h, k, l represents the Miller index of a specific crystal structure and a represents the lattice parameter. Apart from that we need to know the repeat distance. So distance between the 2 lattice point along any direction that follow the similar sequence of atoms. Actually all these elementary (())(76:31) can be useful in (later) discussions on, when you try to discuss in the imperfection or the defects in the crystal structure.

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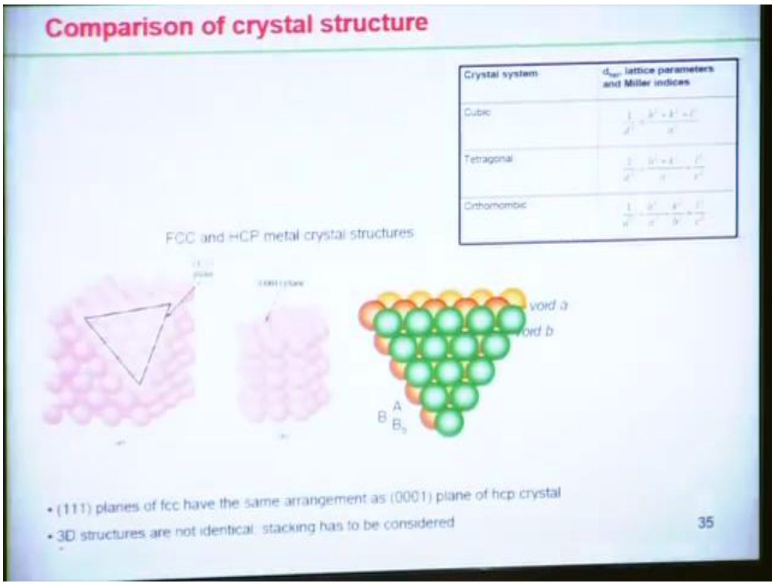

Comparison of crystal structure

Crystal system	d_{hkl}, lattice parameters and Miller indices
Cubic	$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$
Tetragonal	$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$
Orthorhombic	$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$

FCC and HCP metal crystal structures

- (111) planes of fcc have the same arrangement as (0001) plane of hcp crystal
- 3D structures are not identical: stacking has to be considered

So if we look into a comparative analysis of different crystal structure we can see that FCC and HCP there is a almost specific plane of FCC and HCP they are also having a similar kind of arrangement. For example 11 plane of FCC structure and 0 0 0 1 plane of (FCC H) HCP structure actually same arrangement of the crystal generally observed. But 3-D structure is not may not be the identical so it can follow the different stacking sequence; okay that we have already discussed in certain situation and if we look into that crystal system and the the lattice d, we try to estimate the d for the different type of crystal structure we need to know the Miller Indices of a specific plane (and) which is different from the cubic tetragonal and orthorhombic cases.

Okay, so that is all for today. So next we will try to represents the different type of the crystal structure and what are the interstitial sites exist within the crystal structure. Thank you.