INDIAN INSTITUTE OF TECHNOLOGY ROORKEE
NPTEL
NPTEL ONLINE CERTIFICATION COURSE

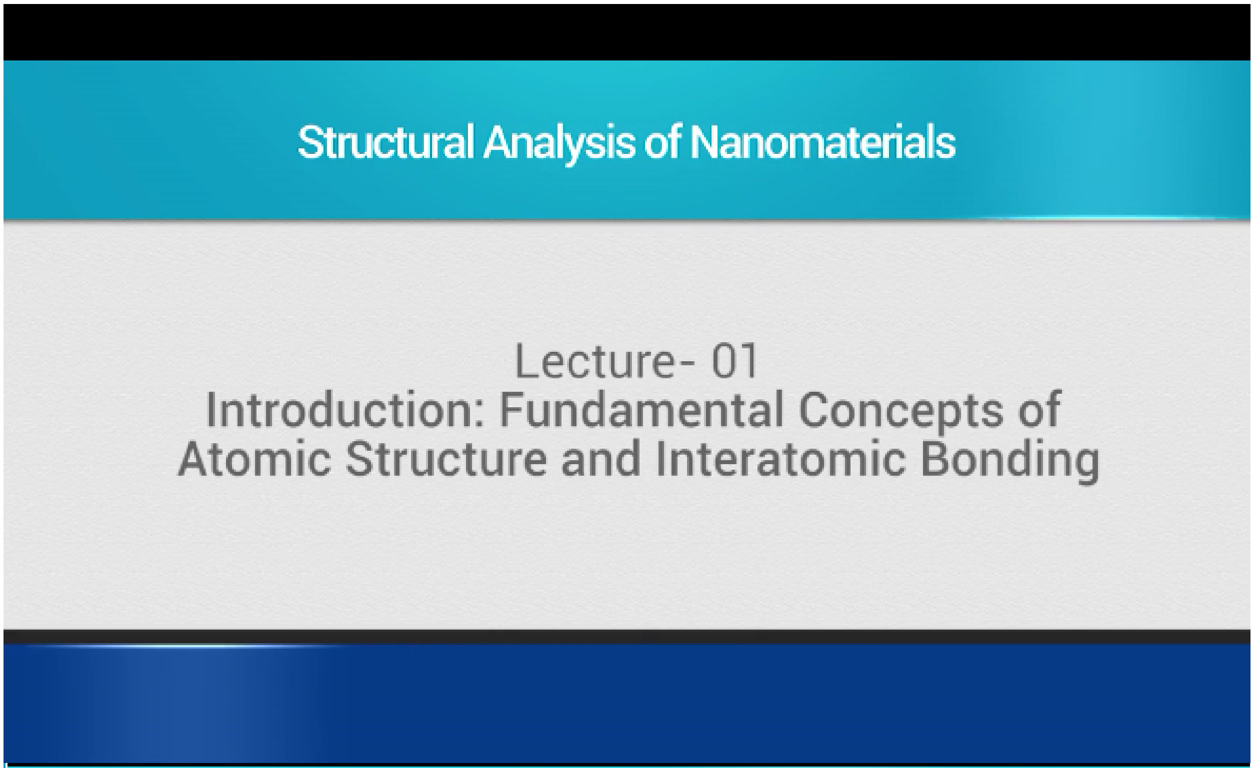
Structural Analysis of Nanomaterials

LECTURE – 01

INTRODUCTION: Fundamental Concepts Of Atomic Structure and Interatomic Bonding

With

Dr. Kaushik Pal
Department of Mechanical & Industrial Engineering
Indian Institute of Technology Roorkee



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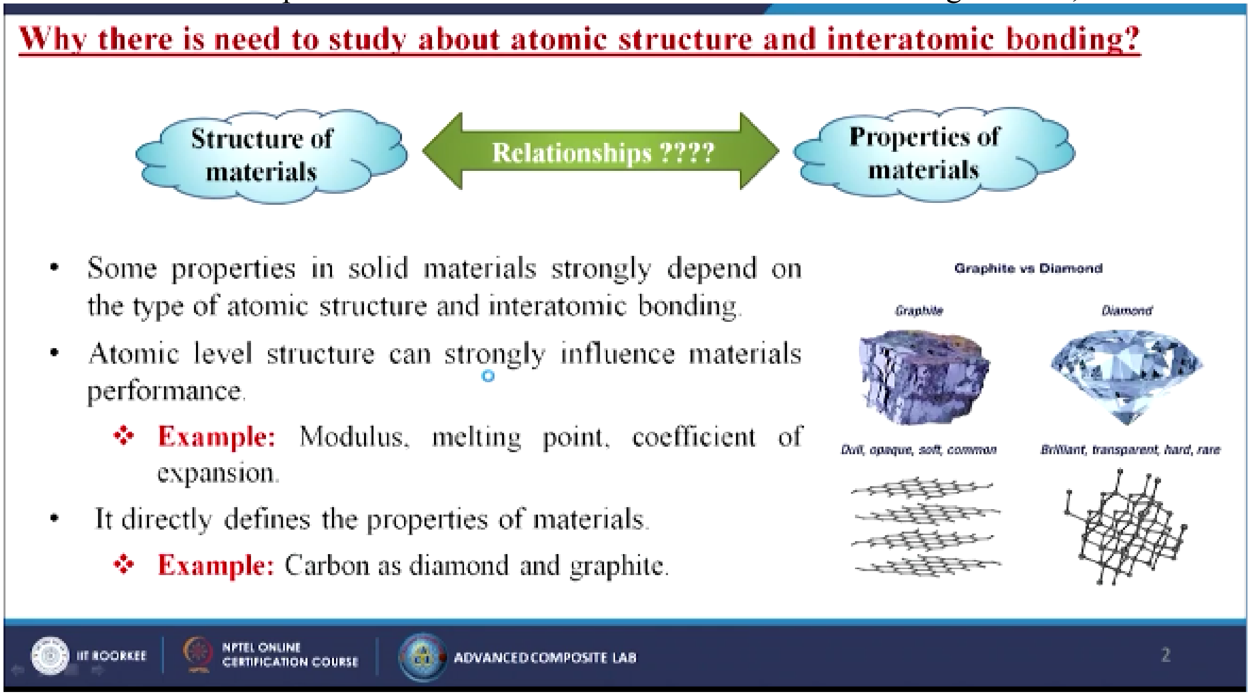
Hello, today actually we are going to start the new lecture on Structural Analysis of Nano materials, this is the broad name of our course that is Structural Analysis of Nano materials, this is very much essential for the scientist, researchers, students or maybe the persons those who are actually dealing the materials in their research or maybe day to day life or maybe making any kind of products.

So generally these objects is a very very essential subjects from which we can get the information about the materials, how they behave and best on their crystal structure, their atomic bonding and also the preparations of the different types of materials and then after that how and the new crystal structure is forming or maybe how they are behaving or maybe whatever the new materials has been formed over there, so and it will also give you the inside picture of that particular materials that how they can behave or maybe they can show their physical properties or maybe the chemical properties or maybe the structural properties.

So basically, actually this chapter is divided into so many sub parts, so first we will discuss about the crystal structure, atomic bonding, then we are going to discuss about the different types of materials like the metals, ceramics, polymers, some kind of advanced materials preparations, and then later we are going to discuss that about the extra that generally by which we can get the informations about the crystal structure of that particular materials, and the last also we are going to give some kind of new techniques like the space or maybe some kind of other methods by which we can get the crystal structure for that particular materials, so simple in a single word I can say that this subject will give a wide informations about the crystal structure and their properties for a particular material.

So today, actually we are going to start our first lecture which is nothing but introduction lecture, so fundamental concepts of atomic structure and there interatomic bonding. So first, before going to start let us know that why it is required to study the atomic structure and the interatomic bonding, so generally in the structure of materials generally what is the relationships when we are getting the properties of materials, so first is the structure of materials, and the properties of materials, and in between the relationships, so relationship will give you the particular essence that how the material will behave, or maybe what kind of material I can add, so what will be the new crystal structure formations, means it is the some kind of, in a single word you can say that, that is a some kind of x-ray kind of view of that particular material from that we can get the informations about the physical properties of that particular materials or maybe about the chemical properties of that particular materials.



Why there is need to study about atomic structure and interatomic bonding?

Structure of materials ⟷ Relationships ???? ⟷ Properties of materials

- Some properties in solid materials strongly depend on the type of atomic structure and interatomic bonding.
- Atomic level structure can strongly influence materials performance.
  - ❖ **Example:** Modulus, melting point, coefficient of expansion.
- It directly defines the properties of materials.
  - ❖ **Example:** Carbon as diamond and graphite.

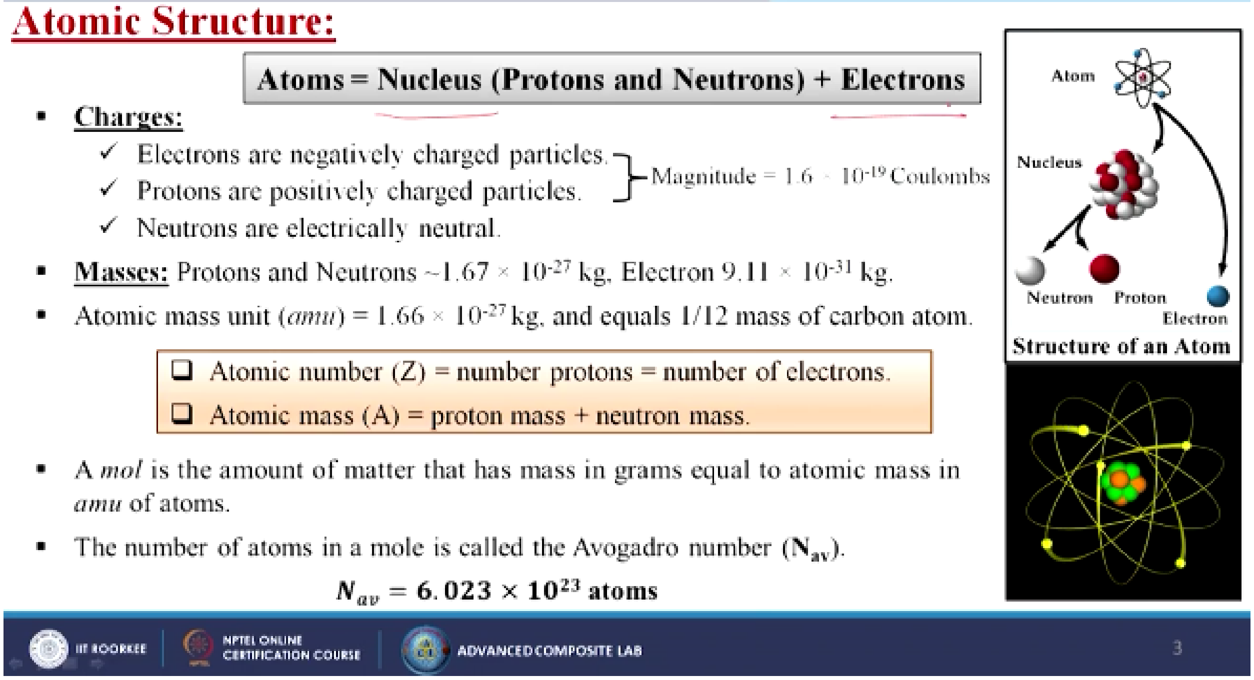
So some properties in solids, strongly depends on that type of atomic structure and the interatomic bonding, these is well known fact, these we have gone to our in class ten standards or maybe class twelve standards, so of course every material is having some atomic structure and the interatomic bonding because the atoms are closely packed with some bonding, otherwise the atom can go randomly anywhere, so there should be some force which can acts in between the atoms, so atomic levels structure can strongly influence the material performance, so this is the vital point over there.

So what are the material performance, generally we can talk about the modulus, we can talk about the melting point, we can talk about the coefficient of the expansion, so it's directly defines the properties of materials is of course from that particular point of view we can get the informations about the materials like carbon as diamond and the graphite.

Here right hand side you can see some kind of things that graphite and diamond we have given the example, so graphite its looks like dull, opaque, soft and the common materials means easily available, when we are talking about the diamond it is very very brilliant, and transparent, and it is having some glittering, or maybe some kind of reflective in nature, it is very hard and it is also the rear earth materials, because it is not easily available, you can prepare it some kind of artificial diamond, but with some help of high end equipment.

So generally you can see the crystal structure of the graphite and you can see the crystal structure of the diamond also, there is some crystal structure of the graphite is the layer by layer stacking, and in the diamond it is a closed packed of the carbon atoms.

So first let us know what is the atomic structure? So generally atoms is equal to nucleus, nucleus is constitute by two things that is the protons and the neutrons and another one is called the electrons, so atom is divided into two groups, one is nucleus, another one is electrons. So here in this atom, so it is the nucleus of that material so it is divided into two parts neutrons and proton which is nothing but the nucleus and another one is coming from electron. So chargers, electrons are negatively charged particles, protons are positively charged particles and neutrons are electrically neutron, so these is the three characteristics of this three.



Atomic Structure:

Atoms = Nucleus (Protons and Neutrons) + Electrons

- **Charges:**
  - ✓ Electrons are negatively charged particles.
  - ✓ Protons are positively charged particles.
  - ✓ Neutrons are electrically neutral.

  Magnitude = 1.6×10^{-19} Coulombs
- **Masses:** Protons and Neutrons ~1.67×10^{-27} kg, Electron 9.11×10^{-31} kg.
- Atomic mass unit (*amu*) = 1.66×10^{-27} kg, and equals 1/12 mass of carbon atom.

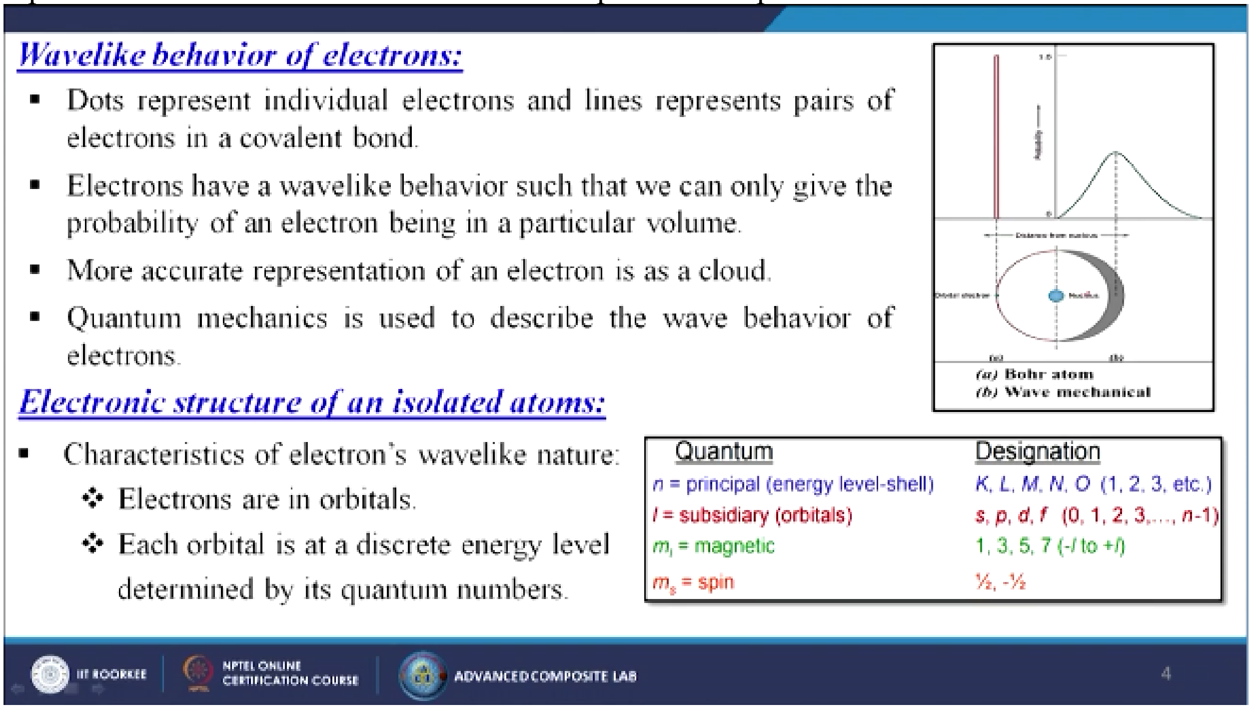
☐ Atomic number (Z) = number protons = number of electrons.
☐ Atomic mass (A) = proton mass + neutron mass.

- A *mol* is the amount of matter that has mass in grams equal to atomic mass in *amu* of atoms.
- The number of atoms in a mole is called the Avogadro number (N_{av}).

$$N_{av} = 6.023 \times 10^{23} \text{ atoms}$$

So what is the magnitude of electrons and protons? Generally 1.6 x 10 to the power -19 coulombs, what is the Masses? Generally protons and neutrons masses are 1.67 x 10 to the power -27 kg, for electron it is 9.11 x 10 to the power -31 kg, what is the atomic mass unit or maybe the AMU? So generally it is 1.66 x 10 to the power -27 kg and equals to 1/12 mass of the carbon atom. So what is the atomic number? Generally it is, generally denoted by number of protons which is equal to number of the electrons.

What is the atomic mass? So generally its proton mass and the neutron mass, so a mole is the amount of matter that has mass in grams equal to atomic mass in AMU of atoms, so the number of atoms in a mole is called the Avogadro number, he is a famous scientist who discovered these numbers and so the, and Avogadro number is 6.023 x 10 to the power 23 atoms. So first let us know the behavior of electron, so generally it's a wavelike behavior so dots in this particular case represents the individual electrons and lines represents the pairs of electrons in a covalent bond, so in this case you can see some dots over there so which is represents the individual electrons, so electrons have a wavelike behavior such that we can only give the probability of an electron being in a particular volume, more accurately presentation of an electron is as a cloud, quantum mechanics is used to describe the wave behavior of electron, generally electronic structure of an isolated atoms, characteristics of the electrons wavelike nature, electrons are in orbitals, each orbital is at a discrete energy level determined by its quantum number, so generally electrons are present and then there is a gap, so the electrons are present in like a orbital, it's like our galaxy, so what is quantum? So generally for n principal energy level, generally we are giving the designations like K, L, M, N, O, like 1, 2, 3, etcetera. For I subsidiary orbitals generally it is S, P, D, F, generally 0, 1, 2, 3, up to the n-1, and for MI magnetic its 1, 3, 5, 7, it's from –I to +I, and MS spin generally it is 1/2 or maybe the -1/2, so these are all the different types of electronic structure.



Wavelike behavior of electrons:

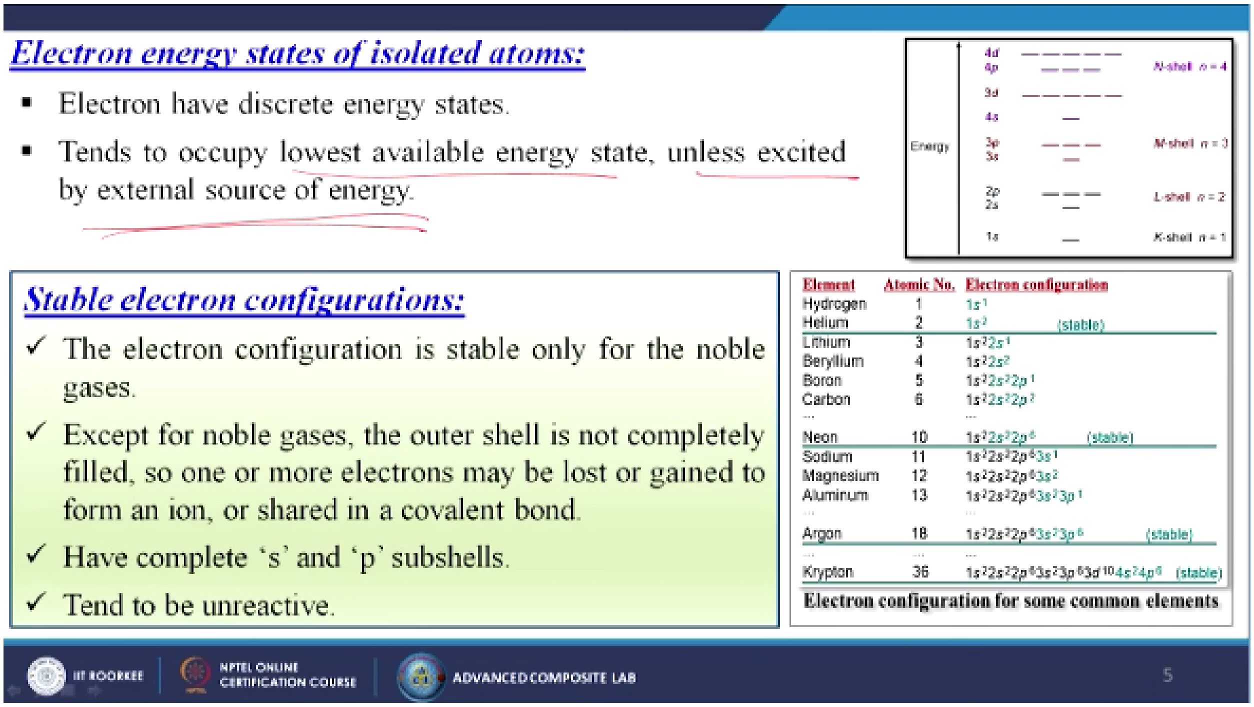
- Dots represent individual electrons and lines represents pairs of electrons in a covalent bond.
- Electrons have a wavelike behavior such that we can only give the probability of an electron being in a particular volume.
- More accurate representation of an electron is as a cloud.
- Quantum mechanics is used to describe the wave behavior of electrons.

(a) Bohr atom
(b) Wave mechanical

Electronic structure of an isolated atoms:

- Characteristics of electron's wavelike nature:
  - Electrons are in orbitals.
  - Each orbital is at a discrete energy level determined by its quantum numbers.

Quantum	Designation
n = principal (energy level-shell)	K, L, M, N, O (1, 2, 3, etc.)
l = subsidiary (orbitals)	s, p, d, f (0, 1, 2, 3,…, n-1)
m_l = magnetic	1, 3, 5, 7 ($-l$ to $+l$)
m_s = spin	½, -½



Electron energy states of isolated atoms:

- Electron have discrete energy states.
- Tends to occupy lowest available energy state, unless excited by external source of energy.

Stable electron configurations:

- ✓ The electron configuration is stable only for the noble gases.
- ✓ Except for noble gases, the outer shell is not completely filled, so one or more electrons may be lost or gained to form an ion, or shared in a covalent bond.
- ✓ Have complete 's' and 'p' subshells.
- ✓ Tend to be unreactive.

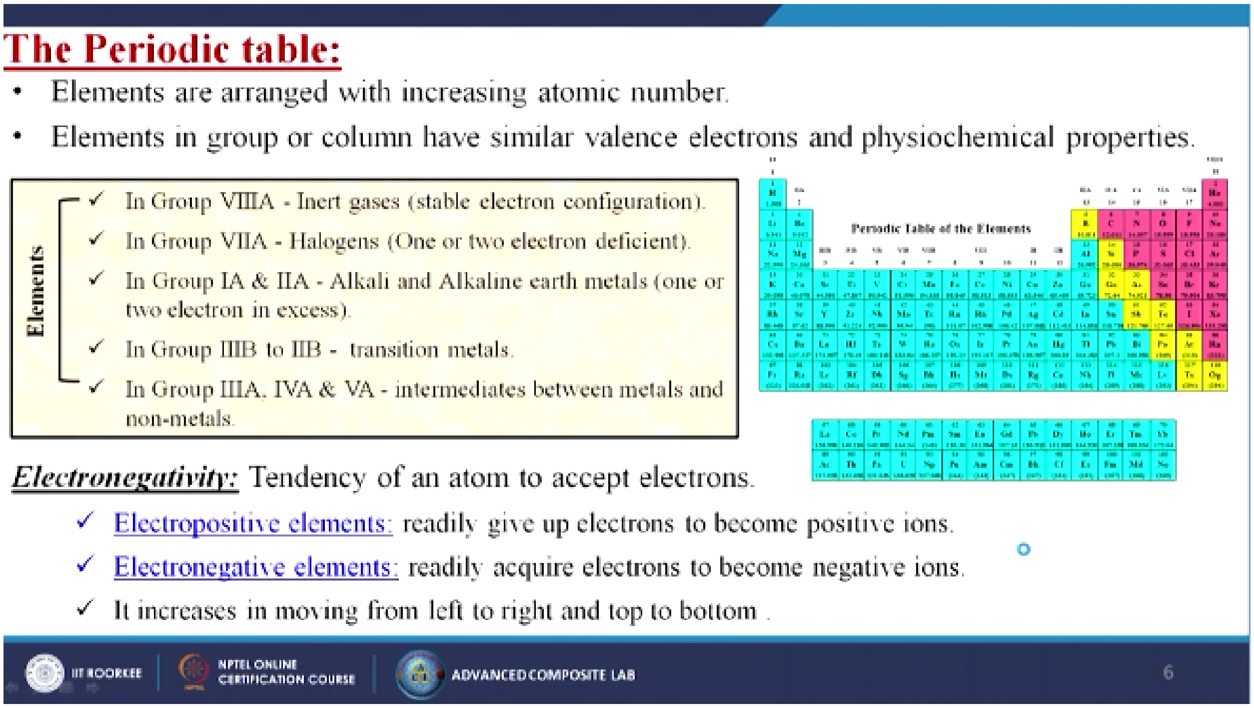
Element	Atomic No.	Electron configuration	
Hydrogen	1	$1s^1$	
Helium	2	$1s^2$	(stable)
Lithium	3	$1s^2 2s^1$	
Beryllium	4	$1s^2 2s^2$	
Boron	5	$1s^2 2s^2 2p^1$	
Carbon	6	$1s^2 2s^2 2p^2$	
...		...	
Neon	10	$1s^2 2s^2 2p^6$	(stable)
Sodium	11	$1s^2 2s^2 2p^6 3s^1$	
Magnesium	12	$1s^2 2s^2 2p^6 3s^2$	
Aluminum	13	$1s^2 2s^2 2p^6 3s^2 3p^1$	
...		...	
Argon	18	$1s^2 2s^2 2p^6 3s^2 3p^6$	(stable)
...	...	...	
Krypton	36	$1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6$	(stable)

Electron configuration for some common elements

So now we are going to discuss about the electron energy states of isolated atoms, so electron have very discrete energy states, tends to occupy lowest available energy state unless excited by the external source of energy, so we have to give the energy to the electron so that the electron can jump from the lower level to the higher level itself, so this is the energy level, so one is it's the k-shell where N =1, and when you are increasing the energy it is going to the up to the 4p or maybe the 4d which is Nth-shell that is N = 4.

So what is the stable electronic configurations? The electron configuration is stable only for the noble gases, except for noble gases the outer shell is not completely filled, because there is some vacancy, so one or more electrons maybe lost or gained to form an ion or shared in a covalent bond, have complete S and P subshells, tend to be very, very unreactive, so here you can see the element and atomic number and the electronic configurations, so for hydrogen generally it is 1S1, for helium it is 1S2 because atomic number is 2, so when we are talking about the say post carbon so it is 6 that means 1S2, 2S2 and 2P2 so it's total 6, when you are talking about the magnesium it's 12, 1S2, 2S2, 2P6 and the 3S2, when we are talking about the argon it is having 18 like 1S2, 2S2, 2P6, 3S2, 3P6 so it's show on.

Now we are going to discuss about the periodic table? So elements are arranged with increasing atomic number, elements in group or column have similar valence electrons and physiochemical



The Periodic table:

- Elements are arranged with increasing atomic number.
- Elements in group or column have similar valence electrons and physiochemical properties.

Elements

- ✓ In Group VIIIA - Inert gases (stable electron configuration).
- ✓ In Group VIIA - Halogens (One or two electron deficient).
- ✓ In Group IA & IIA - Alkali and Alkaline earth metals (one or two electron in excess).
- ✓ In Group IIIB to IIB - transition metals.
- ✓ In Group IIIA, IVA & VA - intermediates between metals and non-metals.

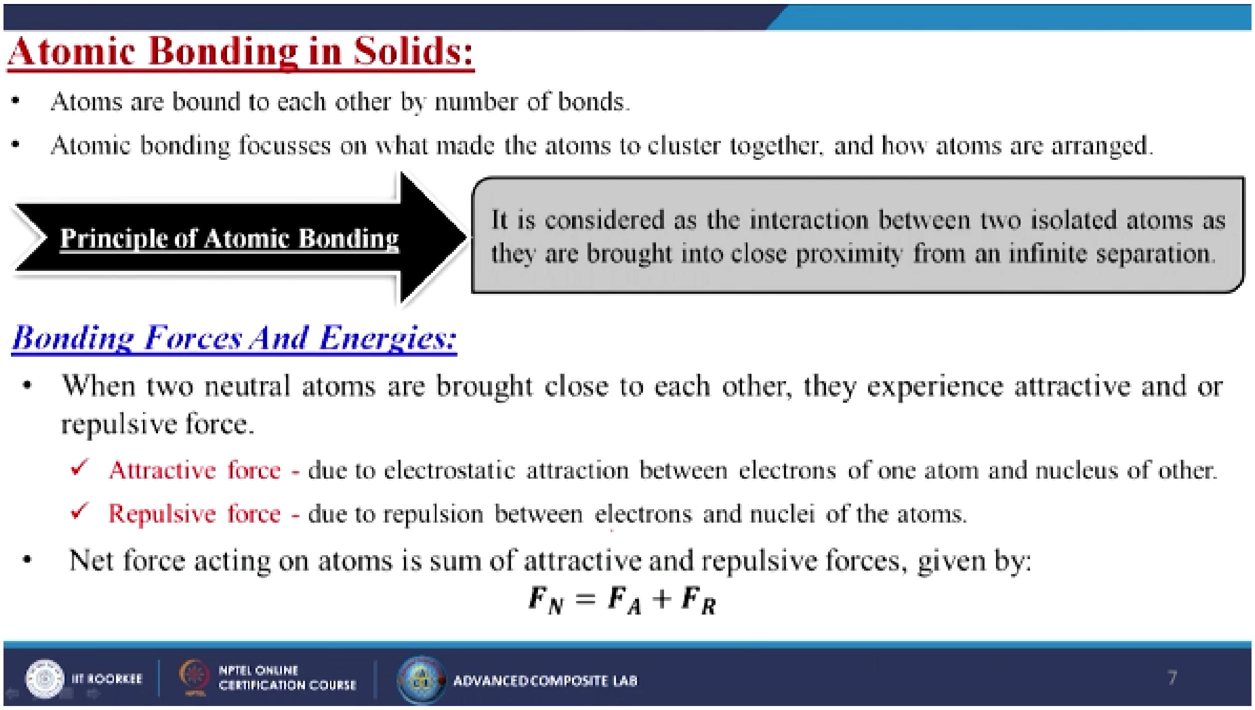
Electronegativity: Tendency of an atom to accept electrons.

- ✓ Electropositive elements: readily give up electrons to become positive ions.
- ✓ Electronegative elements: readily acquire electrons to become negative ions.
- ✓ It increases in moving from left to right and top to bottom .

properties, so elements in group 8A, so if we are talking about the 8, so 8 group or maybe that 8A group in this particular case it is inert gas, so stable electron configurations helium, neon, argon, krypton, xenon, radon, and the OG, so in group 7A so we are talking about the 7A, so here this halogens one or two electrons deficient are there, so like for fluorine, chlorine, bromine, iodine like that, in group 1A and 2A, so when we are talking about 1A and 2A alkali and the alkaline earth metals 1 or 2 electrons in excess like hydrogen, lithium, sodium, potassium, like beryllium, magnesium, calcium like that.

In group 3B and 2B so generally here is that 3B and here is the 2B so in this particular case this all are that transition metals, like strontium, like zinc, like cadmium, like mercury so and so on, in group 3A, 4A, and 5A so in this particular case the 3A, 4A, and 5A so this group so it is the intermediates between metals and non-metals like boron, carbon, nitrogen or maybe aluminum, silicon, phosphorous, gallium, germanium , arsenide, so on.

So what is the electronegativity? Tendency of an atom to accept electrons that’s why it became the negative, so electropositive elements readily give up electrons to become the positive ions, so it is losing the electrons, electronegative elements readily acquired the electrons to become the negative ions, so it is accepting the electrons, it increases in moving from left to right and top to bottom, so it increases in the moving from left to right, and from the top to bottom.



Atomic Bonding in Solids:

- Atoms are bound to each other by number of bonds.
- Atomic bonding focusses on what made the atoms to cluster together, and how atoms are arranged.

Principle of Atomic Bonding

It is considered as the interaction between two isolated atoms as they are brought into close proximity from an infinite separation.

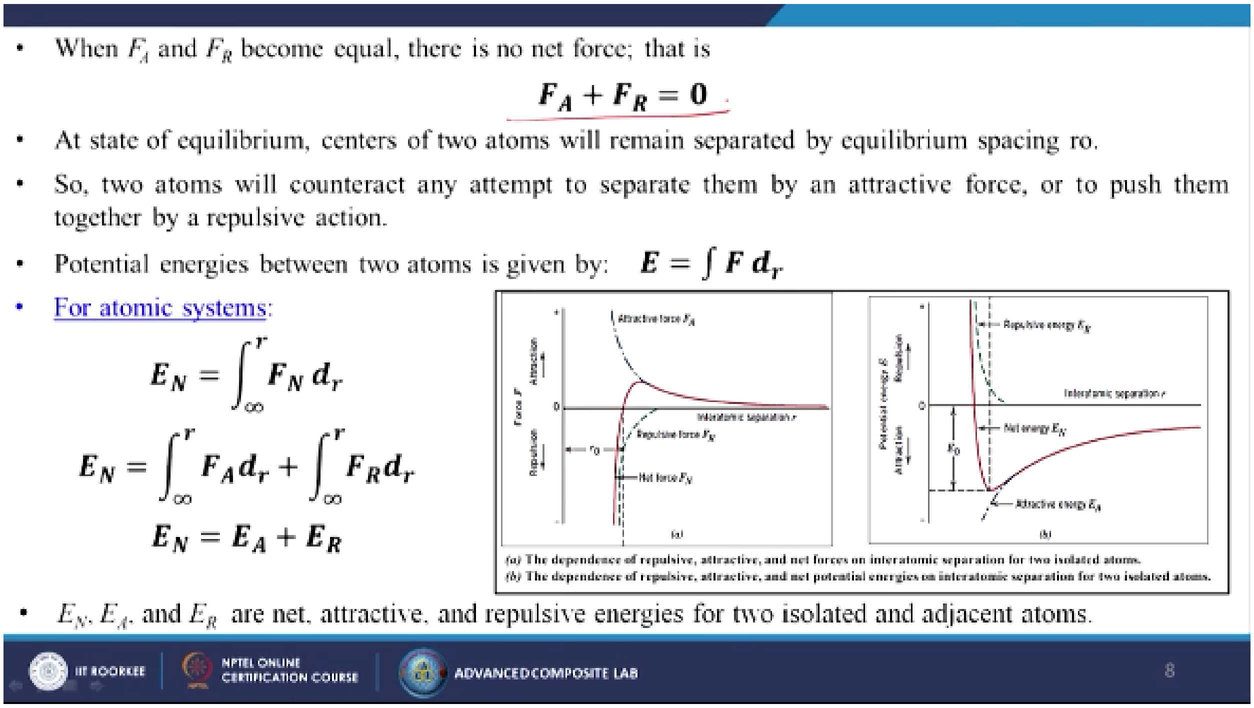
Bonding Forces And Energies:

- When two neutral atoms are brought close to each other, they experience attractive and or repulsive force.
  - ✓ Attractive force - due to electrostatic attraction between electrons of one atom and nucleus of other.
  - ✓ Repulsive force - due to repulsion between electrons and nuclei of the atoms.
- Net force acting on atoms is sum of attractive and repulsive forces, given by:

$$\boldsymbol{F_N = F_A + F_R}$$

Now what is the atomic bonding in solids? So atoms are bound to each other by number of bonds as we already know, so atomic bonding focus on, what made the atoms to cluster together and how atoms are arranged. Yes, as I told already we are having so many atoms so there should be some bonding no, then only the atoms can come close together and give a compact shapes over there, so what is the principle of the atomic bonding, it is considered as the interactions between two isolated atoms as they are brought into close proximity from an infinite separations, so bonding force and about their energies, so when two neutral atoms are brought close to each other, they experience attractive or maybe the repulsive force as we know so it’s like a magnet, so attractive force due to electrostatic attractions between electrons of one atom and nucleus of other.

What is repulsive force? Due to the repulsion between electrons and the nuclei of the atoms itself, so net force acting on atom is sum of the attractive and repulsive force of course which is given by F net is equal to F attraction and the F repulsion, so when FA and FR become equal



- When F_A and F_R become equal, there is no net force; that is

$$F_A + F_R = 0$$

- At state of equilibrium, centers of two atoms will remain separated by equilibrium spacing ro.
- So, two atoms will counteract any attempt to separate them by an attractive force, or to push them together by a repulsive action.
- Potential energies between two atoms is given by: $E = \int F\, d_r$
- For atomic systems:

$$E_N = \int_{\infty}^{r} F_N\, d_r$$

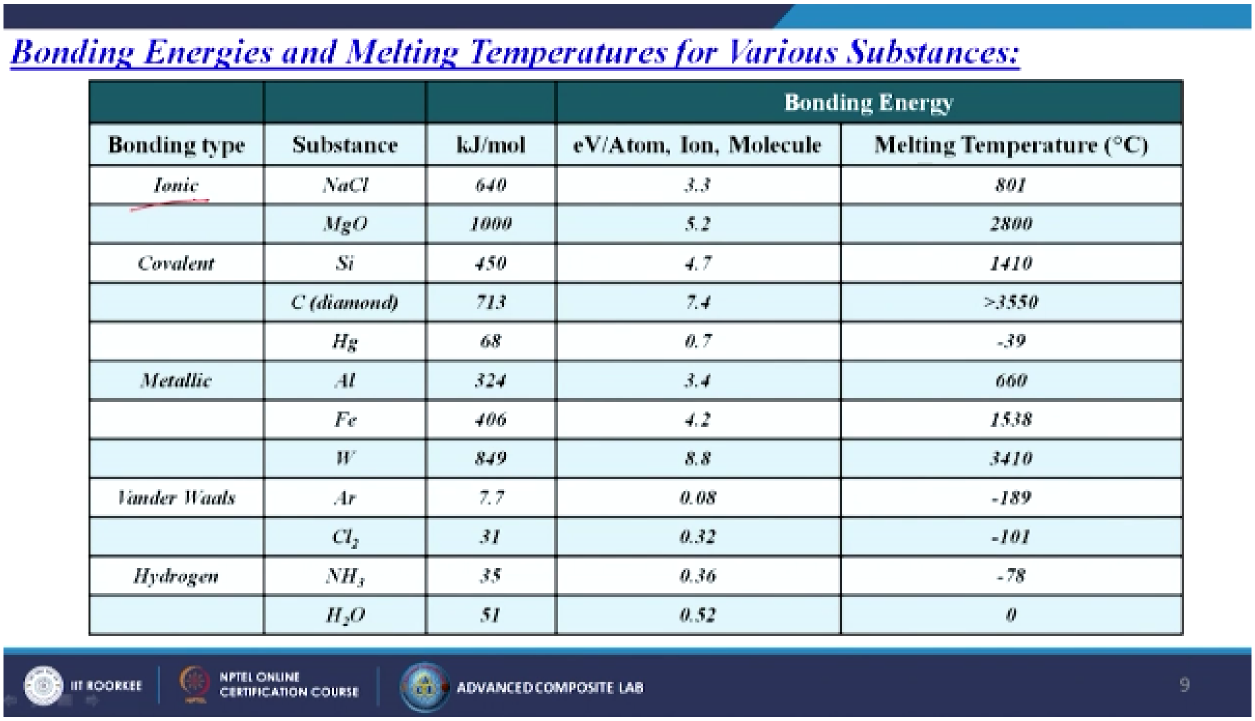
$$E_N = \int_{\infty}^{r} F_A d_r + \int_{\infty}^{r} F_R d_r$$

$$E_N = E_A + E_R$$

(a) The dependence of repulsive, attractive, and net forces on interatomic separation for two isolated atoms.
(b) The dependence of repulsive, attractive, and net potential energies on interatomic separation for two isolated atoms.

- E_N, E_A, and E_R are net, attractive, and repulsive energies for two isolated and adjacent atoms.

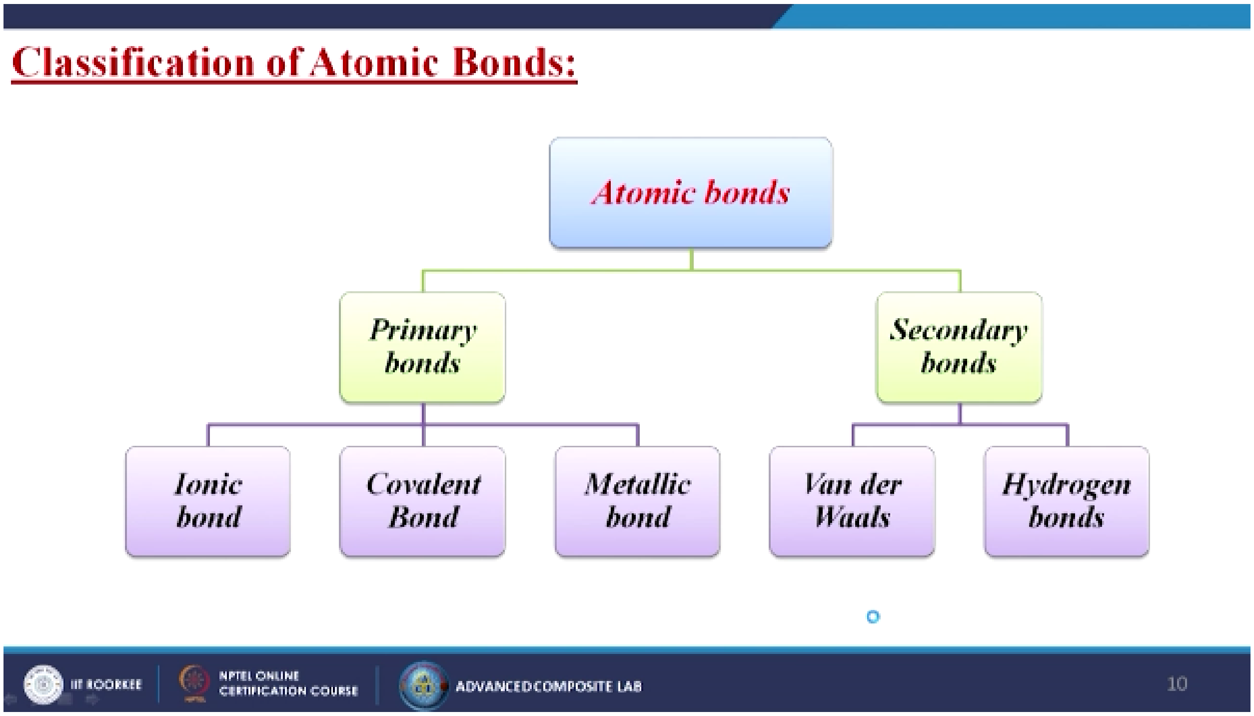
there is no net force that is FA + FR = 0, so as state of equilibrium center of two atoms will remain separated by equilibrium spacing ro, so two atoms will counteract any attempt to separate them by an attractive force or to push them together by a repulsive action, so potential energy between two atoms is given by E is equal to integration FDR, so for atomic systems generally EN is equal to integration infinity to R FN DR which is nothing but the integration, infinity to R FA DR + integration infinity to R FR DR because for the attraction and for the repulsion force that means EN = EA + ER, so here EN, EA and ER are net attractive and the repulsive energies for two isolated and the adjacent atoms, so in this particular case you can see that atomic force is, in this particular case and then the repulsive force and then we are getting the net force here in this particular line, so this is known as the RO, so if we put a tangent over there, so in this particular case also so this is generally for the dependence of the repulsive, attractive, and net force on interatomic separations for two isolated atoms, here the dependence of repulsive attractive and net potential energies on interatomic separations for two isolated atoms.



Bonding Energies and Melting Temperatures for Various Substances:

			Bonding Energy	
Bonding type	**Substance**	**kJ/mol**	**eV/Atom, Ion, Molecule**	**Melting Temperature (°C)**
Ionic	NaCl	640	3.3	801
	MgO	1000	5.2	2800
Covalent	Si	450	4.7	1410
	C (diamond)	713	7.4	>3550
	Hg	68	0.7	-39
Metallic	Al	324	3.4	660
	Fe	406	4.2	1538
	W	849	8.8	3410
Vander Waals	Ar	7.7	0.08	-189
	Cl_2	31	0.32	-101
Hydrogen	NH_3	35	0.36	-78
	H_2O	51	0.52	0

So now we are going to discuss about the bonding energies and melting temperature for various substances, so generally bonding type we are going to know that ionic for like sodium chloride or maybe the magnesium oxide since what is the electron volt per atom on ion or maybe the molecule, what is the bonding energy? It is 3.3, what is the melting temperature? It is 801, when we are talking about the covalent bond, generally silicon or maybe the carbon so it’s bonding energy is 4.7 and melting temperature is 1410, for carbon it is 7.4 and it is more than 3550,when you are talking about the metallic so for generally the metals, metallic bonding so metallic bonding like aluminum it is 3.4 its melting temperature is more than 660 degree centigrade, when we are talking about the Van der Waals bonding or maybe the Van der Waals interactions, so generally for argon it is 0.08 and the melting temperature is -189, it is very, very weak bonding.



Classification of Atomic Bonds:

Atomic bonds

Primary bonds

Secondary bonds

Ionic bond

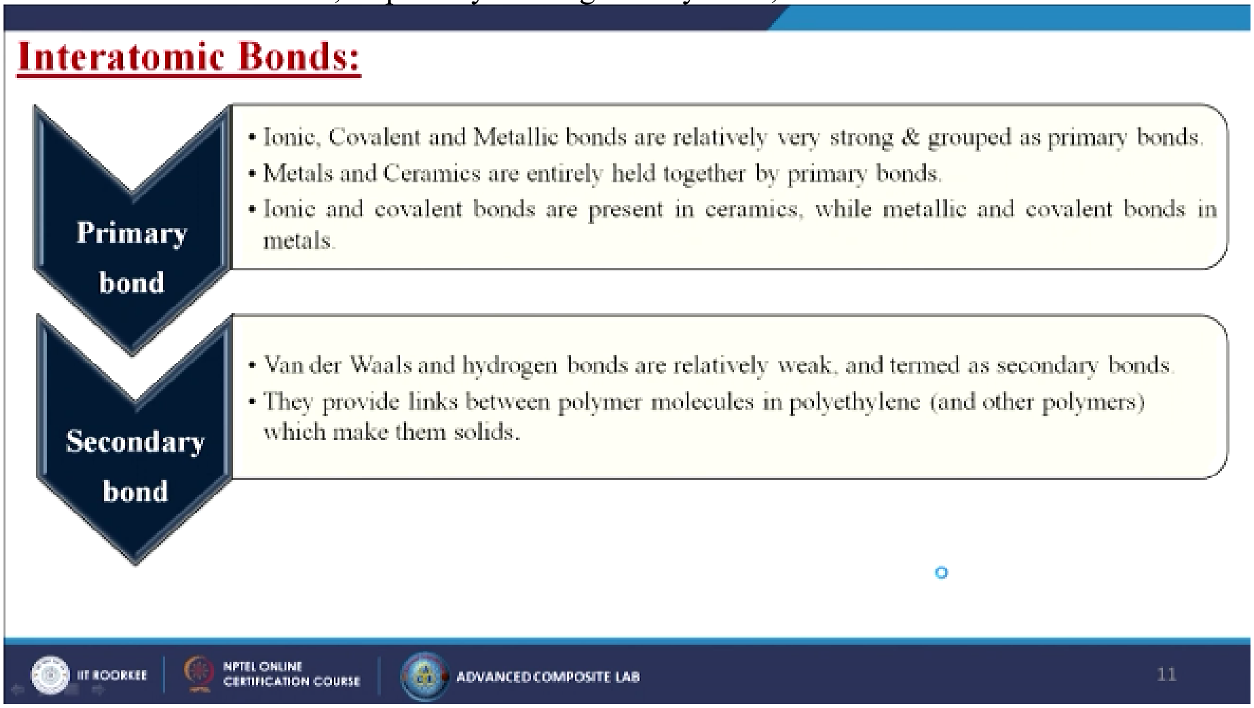
Covalent Bond

Metallic bond

Van der Waals

Hydrogen bonds

When we are talking about the hydrogen bonding generally for the ammonia we are getting it 0.36 and the melting temperature is -78. So now we are going to briefly discuss about the atomic bonds, so generally the atomic bonds has been divided into two parts one is called the primary bonds, another one is called the secondary bonds, so primary bonds is divided into 3 parts that is ionic bond, covalent bond, and the metallic bond, and secondary bonds is two types one is called the Van der Waals bonds or maybe the interactions, another one is called the hydrogen bonds. So what is interatomic bonds, so primary bonds generally ionic, covalent and metallic bonds are



Interatomic Bonds:

Primary bond

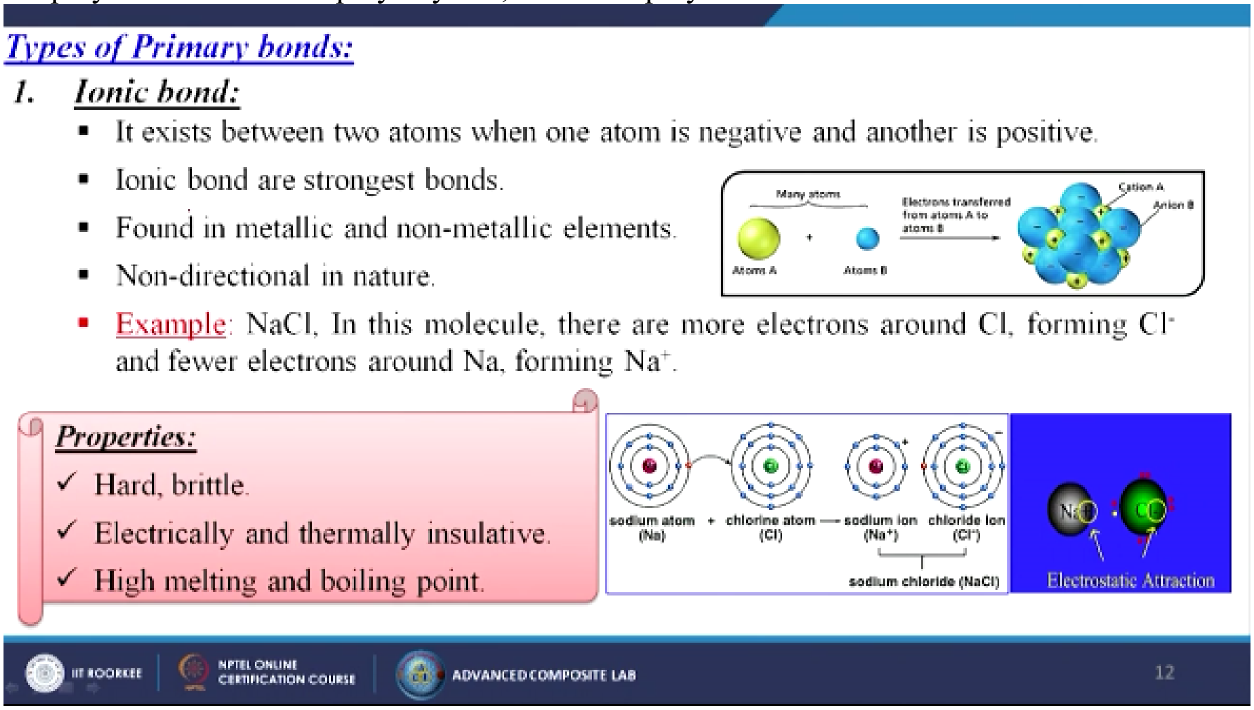
- Ionic, Covalent and Metallic bonds are relatively very strong & grouped as primary bonds.
- Metals and Ceramics are entirely held together by primary bonds.
- Ionic and covalent bonds are present in ceramics, while metallic and covalent bonds in metals.

Secondary bond

- Van der Waals and hydrogen bonds are relatively weak, and termed as secondary bonds.
- They provide links between polymer molecules in polyethylene (and other polymers) which make them solids.

relatively very very strong and grouped as primary bonds, so metals and ceramics are internally held together by the primary bonds itself, ionic and covalent bonds are present in ceramics while metallic and covalent bonds in metals.

So when we are talking about the secondary bond, generally Van der Waals and hydrogen bonds are relatively weak, termed as the secondary bonds as I told already, they provide links between the polymer molecules in polyethylene, and other polymers which make them solid.



Types of Primary bonds:

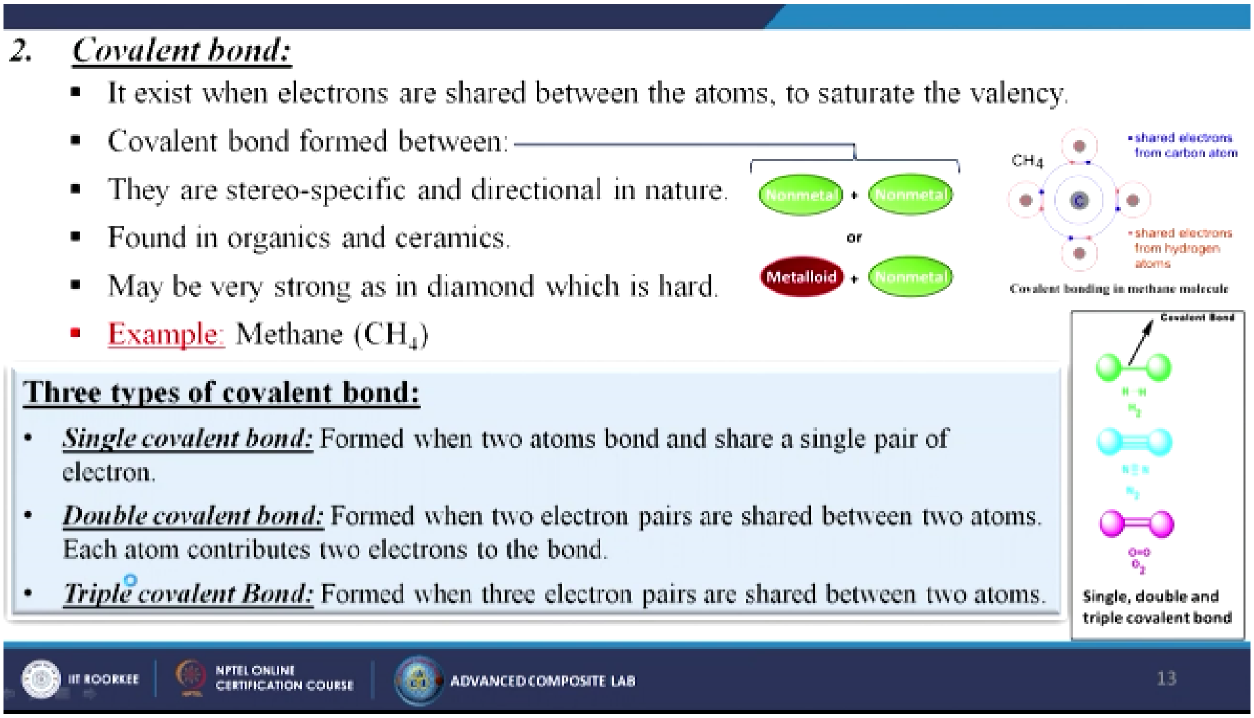
1. Ionic bond:

- It exists between two atoms when one atom is negative and another is positive.
- Ionic bond are strongest bonds.
- Found in metallic and non-metallic elements.
- Non-directional in nature.
- Example: NaCl, In this molecule, there are more electrons around Cl, forming Cl^- and fewer electrons around Na, forming Na^+.

Properties:

- ✓ Hard, brittle.
- ✓ Electrically and thermally insulative.
- ✓ High melting and boiling point.

So now first we’ll discuss about the ionic bonds, so it exists between two atoms when one atom is negative, and another is positive, ionic bonds are the strongest bond, found in metallic and maybe the nonmetallic elements, non-directional in nature so like the best example is that salt sodium chloride, so sodium chloride in this molecule they all are more electrons around chlorine forming CL- and fewer electrons around sodium forming the NA+, so NA+ and CL-, positive and negative. So in this particular case when the sodium is reacting with the chlorine so excess electron is jumping on to the chlorine atom and sodium became the NA+ and the chlorine became the CL-, so it’s like that, so NA+ and the -, some electrostatic attraction is taking place in between that, what is the properties? It is very very hard, brittle in nature, electrically and thermally insulative, high melting and the boiling point.



2. Covalent bond:

- It exist when electrons are shared between the atoms, to saturate the valency.
- Covalent bond formed between:
- They are stereo-specific and directional in nature.
- Found in organics and ceramics.
- May be very strong as in diamond which is hard.
- Example: Methane (CH_4)

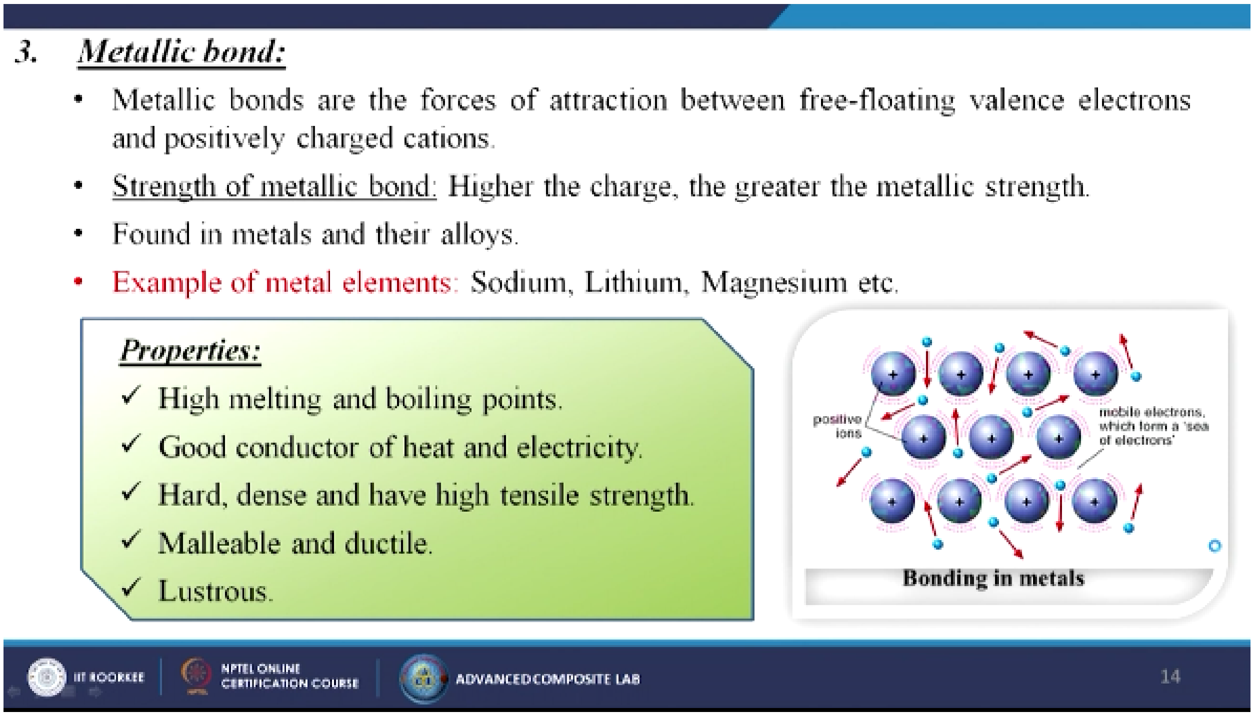
Covalent bonding in methane molecule

Three types of covalent bond:

- ***Single covalent bond:*** Formed when two atoms bond and share a single pair of electron.
- ***Double covalent bond:*** Formed when two electron pairs are shared between two atoms. Each atom contributes two electrons to the bond.
- ***Triple covalent Bond:*** Formed when three electron pairs are shared between two atoms.

Single, double and triple covalent bond

Now we are going to discuss about the covalent bond, it exists when electrons are shared between the atoms to saturate the valency, covalent bond form between non-metal or maybe the non-metal or maybe the metalloid and non-metal, they are stereo specific and directional in nature found in organics and ceramics maybe very strong as in diamond which is very very hard, example is the methane CH4. So in this particular case you can see that C is present in this main orbital and then H is surrounded by this and this all are attached with the covalent bonds, so three types of covalent bonds, first one is called the single covalent bond formed when two atoms bond and share a single pair of electrons. Next double covalent bond formed when two electrons pairs are shared between two atoms, each atom contribute to two electrons to the bond, and the third one is that triple covalent bond formed when three electrons pairs are shared between two atoms.



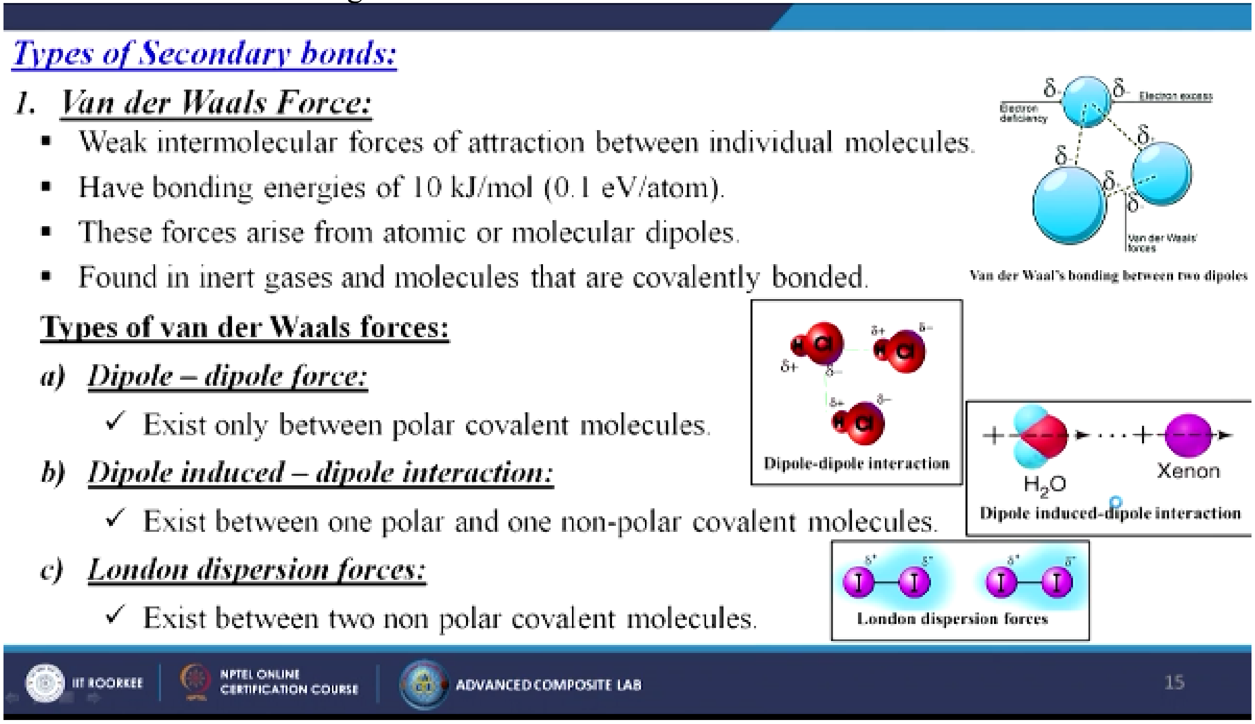
3. *Metallic bond:*

- Metallic bonds are the forces of attraction between free-floating valence electrons and positively charged cations.
- Strength of metallic bond: Higher the charge, the greater the metallic strength.
- Found in metals and their alloys.
- Example of metal elements: Sodium, Lithium, Magnesium etc.

Properties:

- ✓ High melting and boiling points.
- ✓ Good conductor of heat and electricity.
- ✓ Hard, dense and have high tensile strength.
- ✓ Malleable and ductile.
- ✓ Lustrous.

Now we are going to discuss about the metallic bond, metallic bonds are the forces of attractions between free floating, valence electrons and positively charged cations. Strength of metallic bond higher the charge the greater the metallic strength, found in metals and their alloys, example of metal elements like sodium, lithium, magnesium, so what has the properties? Like high melting and boiling points, good conductor of heat and electricity, hard, dense and have tensile strength, malleable and ductile, and it is very, very lustrous means glittering in nature, so here are the bondings in the metals, so due to that ions so generally the mountain bonding are taking place and that should be the charged cations.



Types of Secondary bonds:

1. *Van der Waals Force:*

- Weak intermolecular forces of attraction between individual molecules.
- Have bonding energies of 10 kJ/mol (0.1 eV/atom).
- These forces arise from atomic or molecular dipoles.
- Found in inert gases and molecules that are covalently bonded.

Van der Waal's bonding between two dipoles

Types of van der Waals forces:

a) Dipole – dipole force:

- ✓ Exist only between polar covalent molecules.

Dipole-dipole interaction

b) Dipole induced – dipole interaction:

- ✓ Exist between one polar and one non-polar covalent molecules.

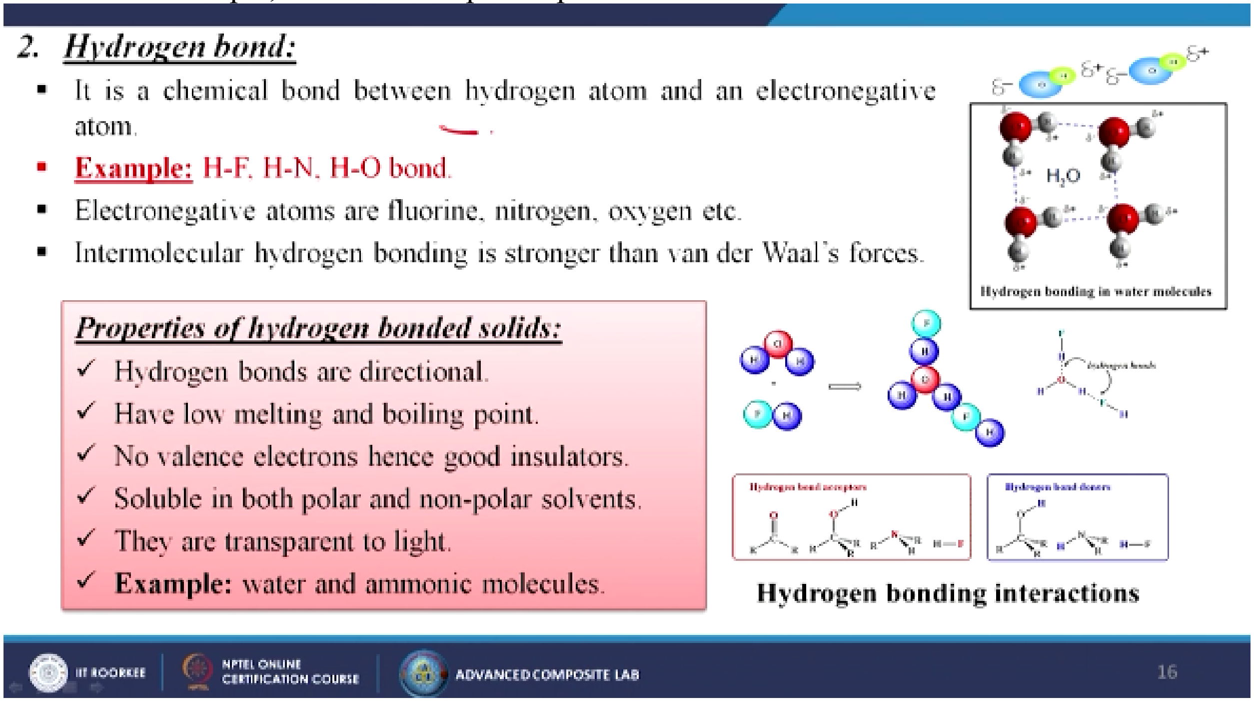
Dipole induced-dipole interaction

c) London dispersion forces:

- ✓ Exist between two non polar covalent molecules.

London dispersion forces

So now we are going to discuss about the types of secondary bonds, first it is the Van der Waals force, it is a very very weak, already I told you that weak intermolecular forces of attractions between the individual molecules have bonding energies of 10 kilo joule per mole it's equivalent to 0.1 electron volt per atom, these forces arise from atomic or molecular dipoles, found in inert gas and molecules that are covalently bonded, so there are three types of generally Van der Waals forces, first one is called the dipole – dipole force exist only between polar covalent molecules, second is dipole induced dipole interaction exist between one polar and one non-polar covalent molecules, and the last one is called the London dispersion forces exist between two non-polar covalent molecules, so this is the London dispersion example, so in this particular case you can see that two non-polar covalent molecules and in between that, it is the dipole induced interactions example, and it is the dipole-dipole interaction.



2. Hydrogen bond:

- It is a chemical bond between hydrogen atom and an electronegative atom.
- **Example:** H-F, H-N, H-O bond.
- Electronegative atoms are fluorine, nitrogen, oxygen etc.
- Intermolecular hydrogen bonding is stronger than van der Waal's forces.

Hydrogen bonding in water molecules

Properties of hydrogen bonded solids:

- ✓ Hydrogen bonds are directional.
- ✓ Have low melting and boiling point.
- ✓ No valence electrons hence good insulators.
- ✓ Soluble in both polar and non-polar solvents.
- ✓ They are transparent to light.
- ✓ **Example:** water and ammonic molecules.

Hydrogen bonding interactions

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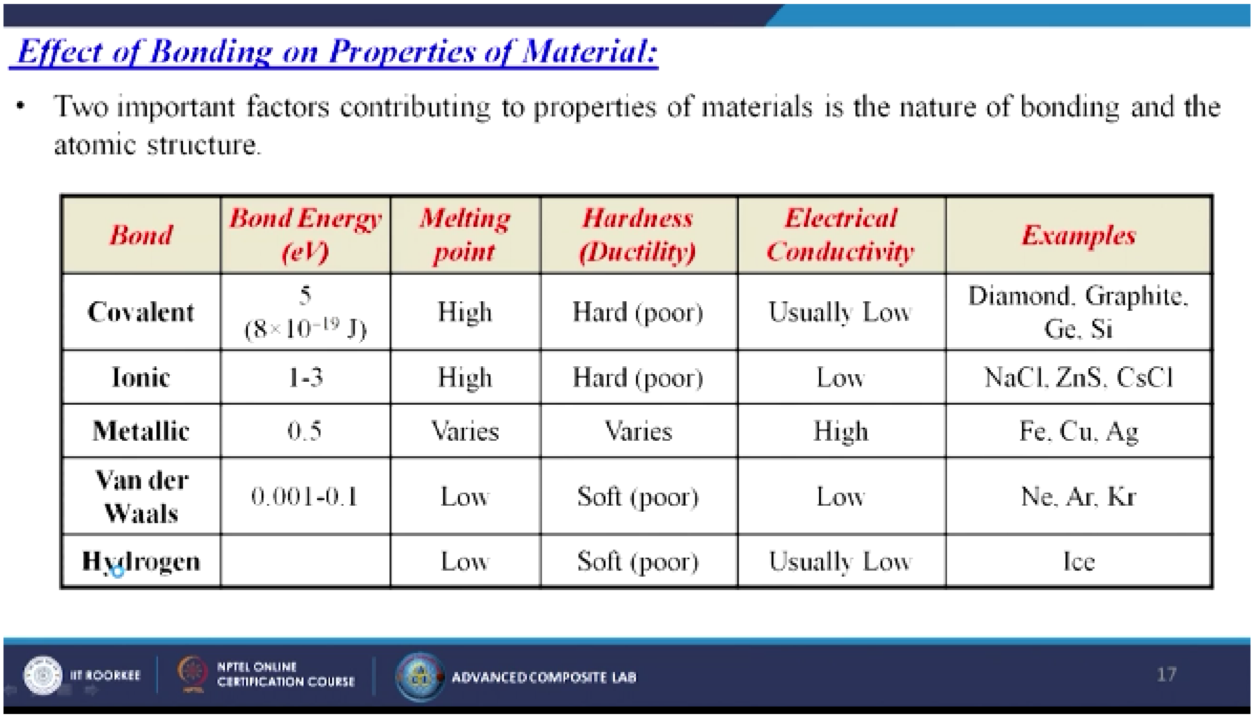
Next we are going to discuss about the hydrogen bond, it is a chemical bond between hydrogen atom and an electronegative atom generally we can find it like HF, HN, HO bond generally it is called the hydrogen bond, electronegative atoms are fluorine, nitrogen, oxygen, intermolecular hydrogen bonding is stronger than the Van der Waals force. So properties of the hydrogen bond, so hydrogen bonds are directional so have low melting and boiling point, low valence electrons hence could insulators, so soluble in both polar and the non-polar solvents, they are transparent to the light, example, best example is the water and the some ammonic molecules.

So now we are going to discuss about the effects of bonding on the properties of materials, how it effects, two important factors contributing to properties of materials is the nature of bonding

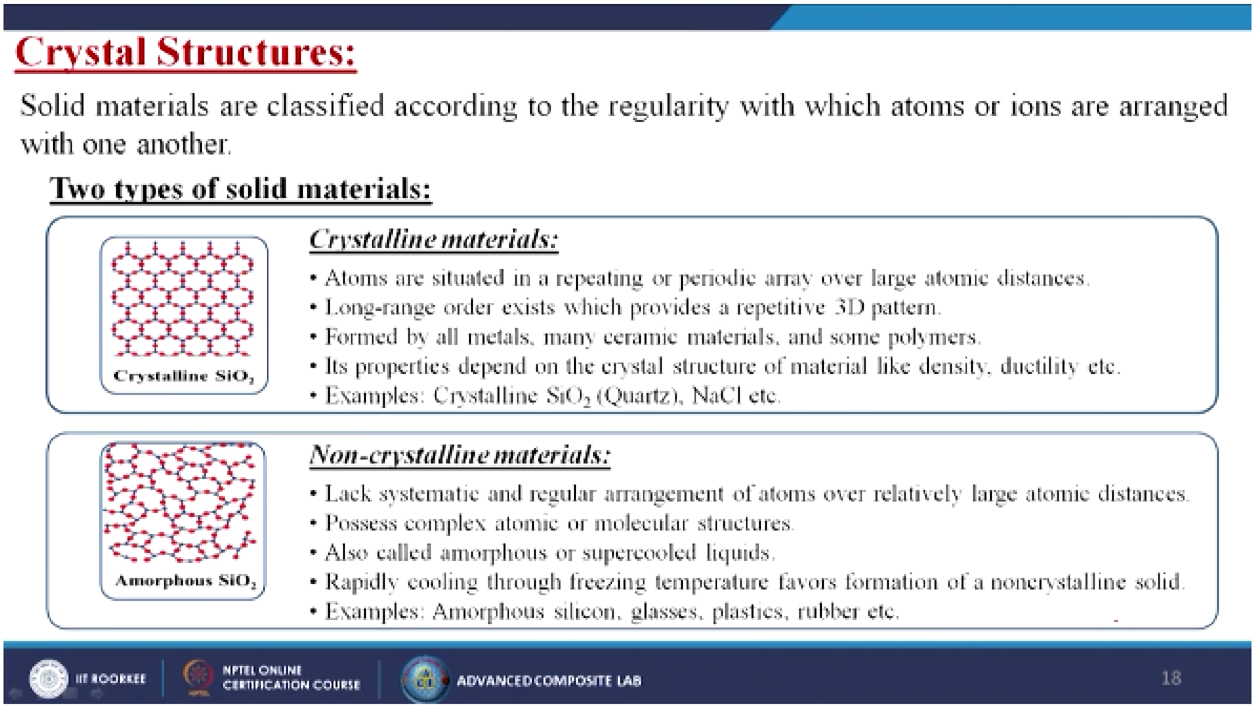


Effect of Bonding on Properties of Material:

- Two important factors contributing to properties of materials is the nature of bonding and the atomic structure.

Bond	Bond Energy (eV)	Melting point	Hardness (Ductility)	Electrical Conductivity	Examples
Covalent	5 (8×10^{-19} J)	High	Hard (poor)	Usually Low	Diamond, Graphite, Ge, Si
Ionic	1-3	High	Hard (poor)	Low	NaCl, ZnS, CsCl
Metallic	0.5	Varies	Varies	High	Fe, Cu, Ag
Van der Waals	0.001-0.1	Low	Soft (poor)	Low	Ne, Ar, Kr
Hydrogen		Low	Soft (poor)	Usually Low	Ice

and of course the atomic structure, so first we are going to discuss the covalent bond, so bond energy is 5 electron volt melting point is high, hardness in terms of ductility it is hard, and ductility is very, very poor, electrical conductivity is very low, and the examples diamond, graphite, germanium, silicon, its ionic, generally the bond energy is 1, 2, 3, melting point is high, it's hardness is hard, ductility is very very poor, electrical conductivity is low like sodium chloride, zinc sulfite and the CACL, so when you are talking about the metallic, it's 0.5 electron volt, it's melting point varies, hardness also varies and electrical conductivity is very very high like iron, copper, silver, etcetera, Van der Waals force it varies from 0.001 to 0.1, melting point is low, then hardness is soft but ductility is also very poor, electrical conductivity is also low like neon, argon, krypton, like that, and last one is the hydrogen, it's melting point is very very low, hardness is soft, and ductility is poor, usually low and generally the example is the ice or maybe the water.



Crystal Structures:

Solid materials are classified according to the regularity with which atoms or ions are arranged with one another.

Two types of solid materials:

Crystalline SiO_2

Crystalline materials:

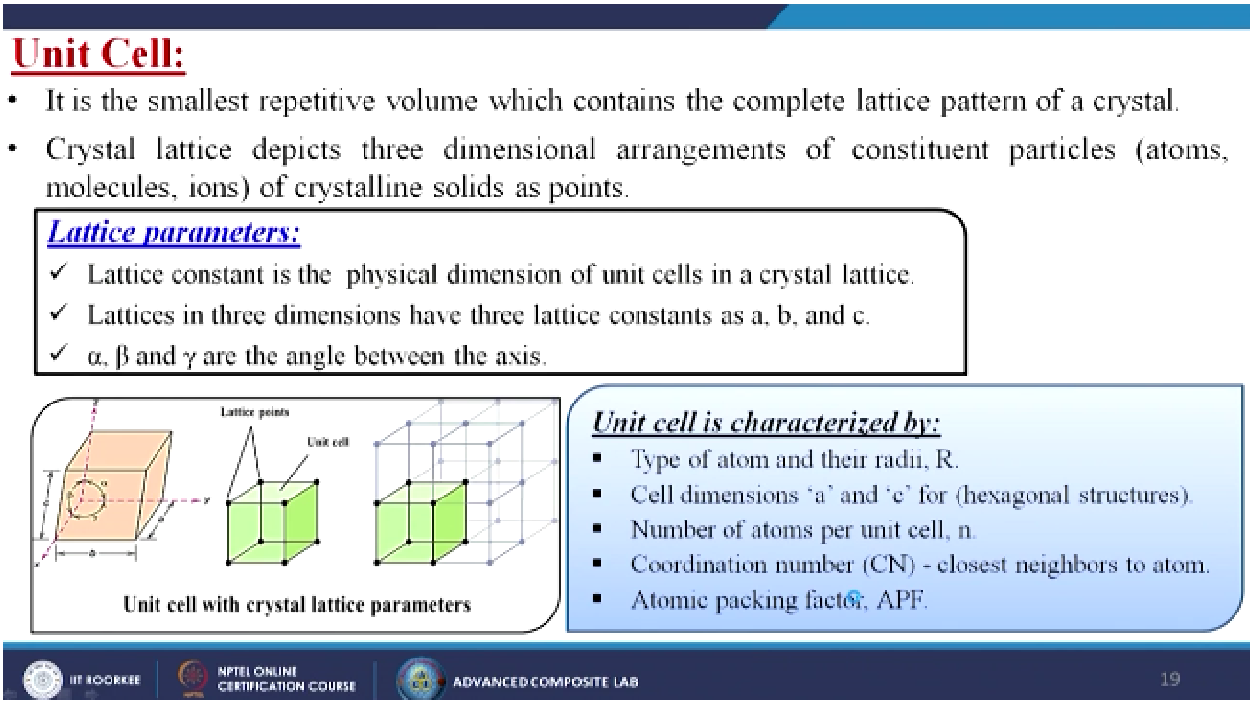
- Atoms are situated in a repeating or periodic array over large atomic distances.
- Long-range order exists which provides a repetitive 3D pattern.
- Formed by all metals, many ceramic materials, and some polymers.
- Its properties depend on the crystal structure of material like density, ductility etc.
- Examples: Crystalline SiO_2 (Quartz), NaCl etc.

Amorphous SiO_2

Non-crystalline materials:

- Lack systematic and regular arrangement of atoms over relatively large atomic distances.
- Possess complex atomic or molecular structures.
- Also called amorphous or supercooled liquids.
- Rapidly cooling through freezing temperature favors formation of a noncrystalline solid.
- Examples: Amorphous silicon, glasses, plastics, rubber etc.

Now we are going to discuss about the crystal structure, so solid materials are classified according to the regularity with which atoms or ions are arranged with one another, two types of solid materials generally one is called the crystalline materials, another one is called the non-crystalline materials, so what is the crystalline materials? Atoms are situated in a repeating or periodic array over large atomic distances. Long range order exists which provides a repetitive 3D pattern, formed by all metals, many ceramic materials and some polymers, its properties depend on the crystal structure of materials like density, ductility, etcetera, examples crystalline silicon dioxide generally known as Quartz, sodium chloride so you can see that crystalline silicon dioxide crystal structure. Then we are going to discuss about the non-crystalline materials, so it’s having very lack systematic and regular arrangement of atoms over a relatively large atomic distances, possess complex atomic or molecular structures also called the amorphous or maybe the super cooled liquids, rapidly cooling through freezing temperature favors formation of a non-crystalline solids, what is the example, amorphous silicon, glasses, plastics, rubber etcetera.



Unit Cell:

- It is the smallest repetitive volume which contains the complete lattice pattern of a crystal.
- Crystal lattice depicts three dimensional arrangements of constituent particles (atoms, molecules, ions) of crystalline solids as points.

Lattice parameters:

- ✓ Lattice constant is the physical dimension of unit cells in a crystal lattice.
- ✓ Lattices in three dimensions have three lattice constants as a, b, and c.
- ✓ α, β and γ are the angle between the axis.

Unit cell with crystal lattice parameters

Unit cell is characterized by:

- ▪ Type of atom and their radii, R.
- ▪ Cell dimensions 'a' and 'c' for (hexagonal structures).
- ▪ Number of atoms per unit cell, n.
- ▪ Coordination number (CN) - closest neighbors to atom.
- ▪ Atomic packing factor, APF.

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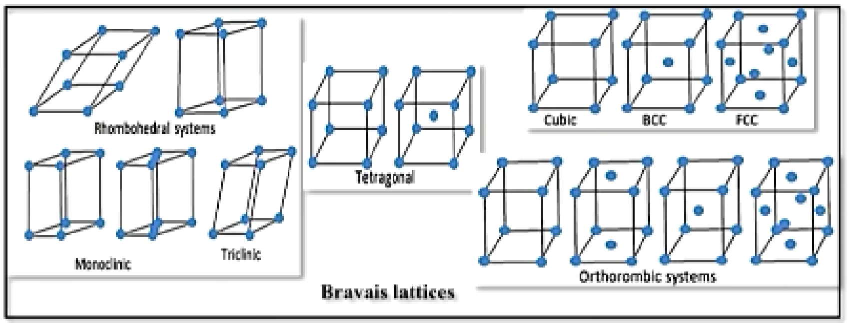
Now we are going to discuss one very interesting thing that is called the unit cell, so it is the smallest repetitive volume which contains the complete lattice pattern of a crystal, so it is the one, you can say one small backbone kind of things, so crystal lattice depicts 3 dimensional arrangements of constituent particles like atoms, molecules and the ions of crystalline solids as point.

Lattice parameter, lattice constant is the physical dimension of unit cell in a crystal lattice, these part I will briefly discuss in the subsequent lecture, lattice in 3 dimensions have 3 lattice parameters like A, B, and C, alpha, beta and gamma are the angle between the axis, so if you see the lattice parameters so here these angle is alpha, then this is beta, and this is the gamma 1, so lattice point this is the unit cells, so this is denoting by A, this is B, and this is C, if it is the cubic 1 then A = B = C, so generally unit cell is characterize by type of atom and they are ready or cell dimensions A and C for the hexagonal structures, number of atoms per unit cell that is n, coordination number that closest neighbor to atoms and atomic packing factor that is APF, these all in brief I am going to discuss into the second lecture.

Crystal Systems:

- Based on length equality or inequality and their orientation (the angles between them, α, β and γ) a total of 7 crystal systems are defined.
- Seven crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, triclinic 2 monoclinic.
- Total 14 Bravais lattices fall into seven crystal system.



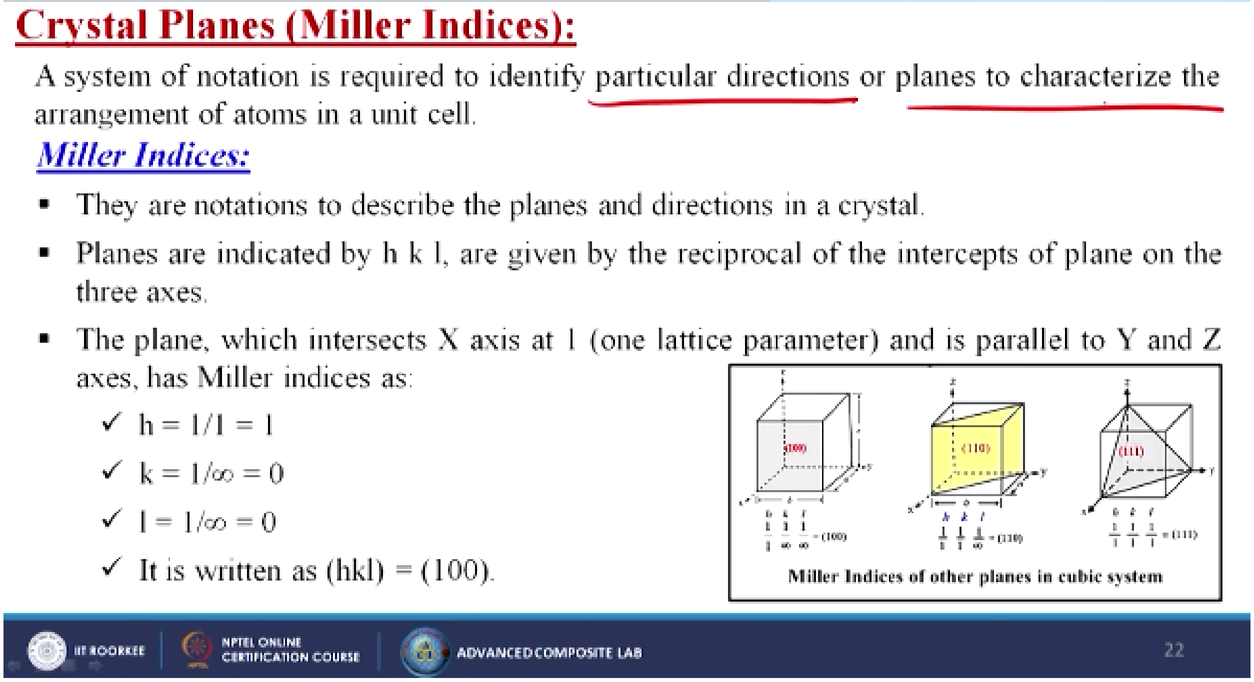
Bravais lattices

So what is the crystal systems, best on length equality or inequality and there orientations, the angles between them alpha, beta and gamma, a total of 7 crystal systems are defined, 7 crystal systems are cubic, tetragonal, hexagonal, orthorhombic, rhombohedral, triclinic 2 monoclinic, total 14 Bravais lattice fall into 7 crystal systems, so this is the example of the rhombohedral systems, monoclinic and the triclinic, then tetragonal, then cubic like BCC body center cubic, FCC face center cubic, this is the orthorhombic systems, so total these all are the different types of Bravais lattices.

Different crystal systems with axial length and angle:

Crystal system	Axial length	Angle	Bravais lattice
Cubic	a = b = c	α = β = γ =90°	Simple Body-centered Face-centered
Tetragonal	a = b ≠ c	α = β = γ =90°	Simple Body-centered
Orthorhombic	a ≠ b ≠ c	α = β = γ =90°	Simple Body-centered Face-centered
Rhombohedral	a = b = c	α = β = γ ≠ 90°	Simple
Hexagonal	a = b ≠ c	α = β = 90° , γ =120°	Simple Hexagonal close-packed
Monoclinic	a ≠ b ≠ c	α = γ = 90° ≠ β	Simple
Triclinic	a ≠ b ≠ c	α ≠ β ≠ γ ≠ 90°	Simple

So now we are going to discuss about the different crystal systems with axial length and the angle, so for generally cubic as I told already it is A = B = C because all the length are same because it is cubic, angle it's perfectly 90 degree to each other so alpha = beta = gamma = 90 degree. Bravais lattice it is simple, generally sometimes it is body centered, sometime it is face centered also. When we are talking about the tetragonal, it's A = B not is equal to C, alpha, beta, gamma = 90 degree, generally it is simple and the body centered one.
Orthorhombic A not equal B, not equal to C = alpha = beta and gamma all are 90 degree, it is simple, body centered and the face centered. When we are talking about the rhombohedral A = B = C, alpha, beta and gamma are not 90 degree it is simple, it is hexagonal, A = B, but not is equal to C, alpha beta is 90 degree but gamma is 120 degree, it is simple, hexagonal close packed. Then monoclinic A not equal to B, not equal to C, alpha = gamma = 90 degree but not the beta it is simple. Next one is the triclinic, it is A not equal to B, not equal to C, alpha not equal to beta, not equal to gamma, not equal to 90 degree it is very, very simple.



Crystal Planes (Miller Indices):

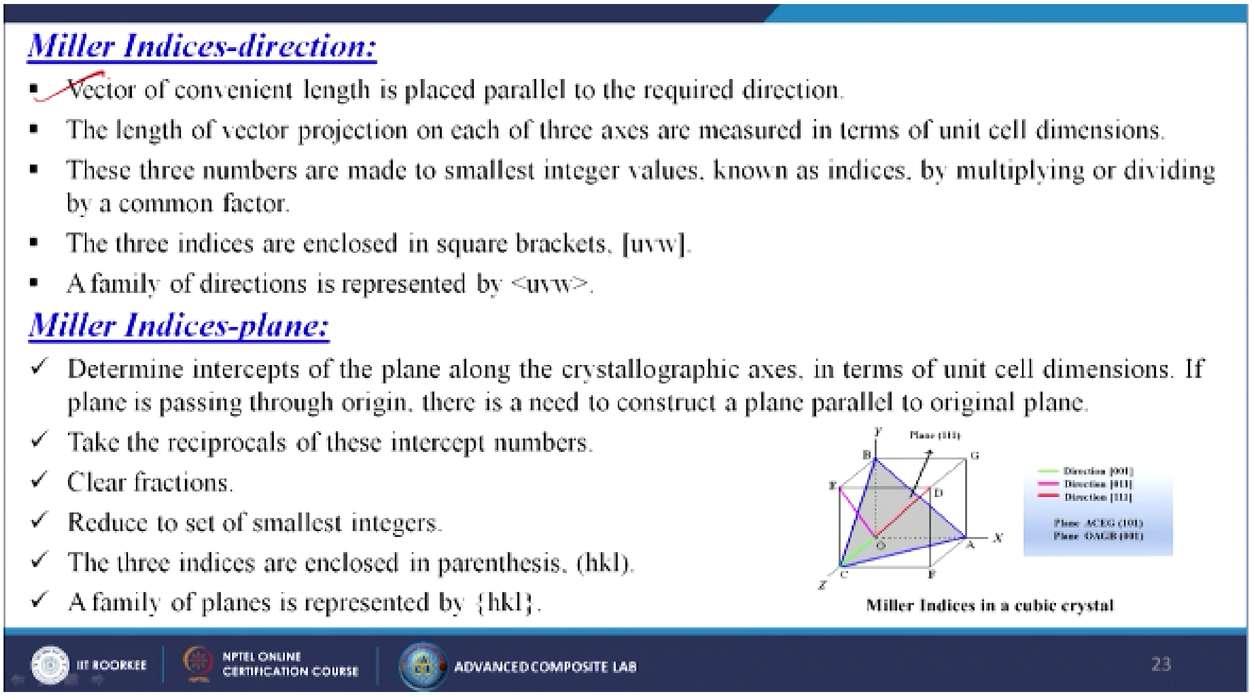
A system of notation is required to identify particular directions or planes to characterize the arrangement of atoms in a unit cell.

Miller Indices:

- They are notations to describe the planes and directions in a crystal.
- Planes are indicated by h k l, are given by the reciprocal of the intercepts of plane on the three axes.
- The plane, which intersects X axis at 1 (one lattice parameter) and is parallel to Y and Z axes, has Miller indices as:
  - ✓ h = 1/1 = 1
  - ✓ k = 1/∞ = 0
  - ✓ l = 1/∞ = 0
  - ✓ It is written as (hkl) = (100).

Miller Indices of other planes in cubic system

So now we are going to discuss about the crystal planes that is Miller indices, a system of notations is required to identify the particular directions or planes to characterize the arrangement of atoms in a unit cell. Now it is the very interesting one that is called the Miller indices, so they are the notations to describe the planes and the directions in a crystal, planes are directed by H K L are given by the reciprocal of the intercepts of plane on the three axes, so 1/H, 1/K and 1/L, so the plane which intersects X axis at 1, 1 lattice parameter and is parallel to Y and Z axes has Miller indices like H = 1/1 = 1, K = 1/infinity = 0, and L = 1/infinity = 0, so it will be written as HKL value 1 0 0, so in this particular case so you are having X =1, so this is your starting point, so from this you will come, so you will come 1 unit over here, and then your K and L value is almost 0, so Y and 0 so you were talking about these plane itself, so that is the 1 0 0 plane.



Miller Indices-direction:

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

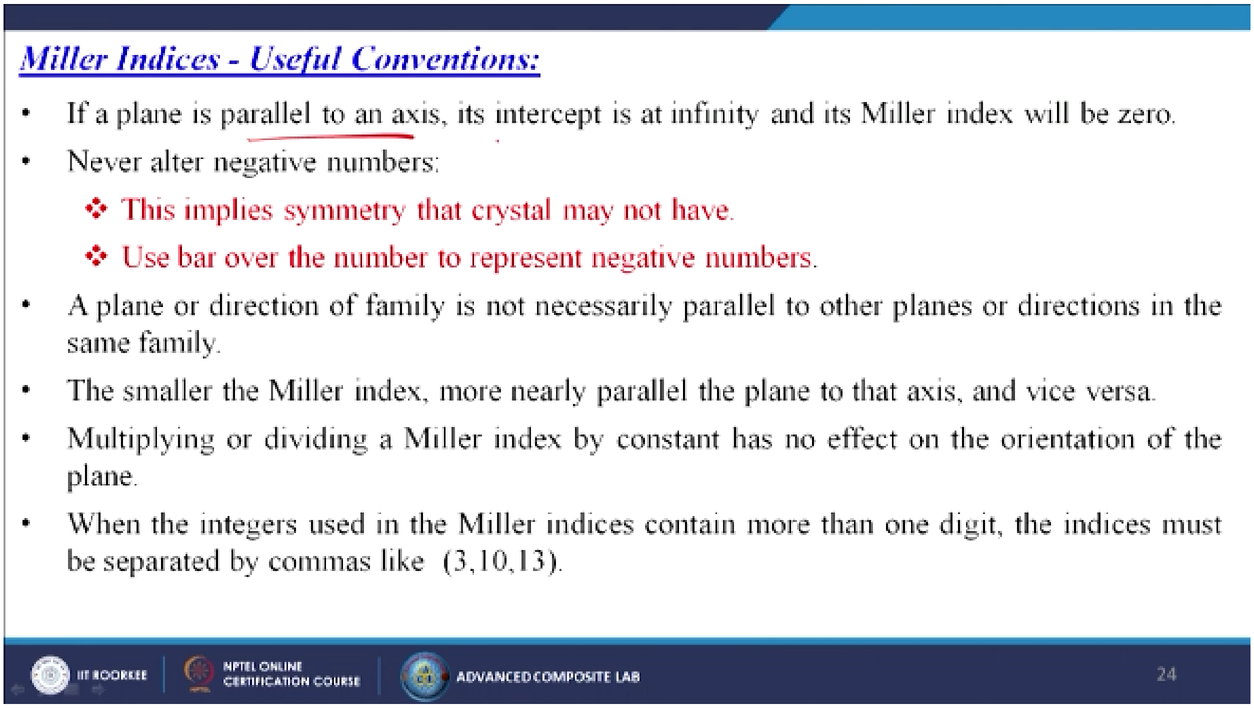
Miller Indices-plane:

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

Miller Indices in a cubic crystal

Then you are coming to 1 and then your L is also 1 is going, but this is 0 so you are talking about this plane itself that is 1 1 0 plane, and 1 1 1 is this plane only, so this is known as the 1 1 plane, so like this way we can calculate the total plane of that particular crystal structure. So Miller indices directions, vector of convenient length is placed parallel to the required directions, the length of vector projection on each of three axes are measured in terms of the unit cell dimensions. These three numbers are made to smallest integer value known as indices by multiplying or dividing by a common factor. The three indices are enclosed in square brackets like this way in the third brackets UVW, a family of directions is represented by in this manner, so less than UVW greater than.

Now we are going to discuss about the Miller indices-plane, so determine intercepts of the plane along the crystallographic axes in terms of unit cell dimensions, if plane is passing through the origin there is a need to construct a plane parallel to the original plane, so take the reciprocals of these intercept numbers, so first you are making a plane, so it is passed through the origin itself, so now take the reciprocals of these intercept numbers, clear fractions, reduced to set of smallest integers, the three integers are enclosed in parenthesis like within flower bracket HKL, a family



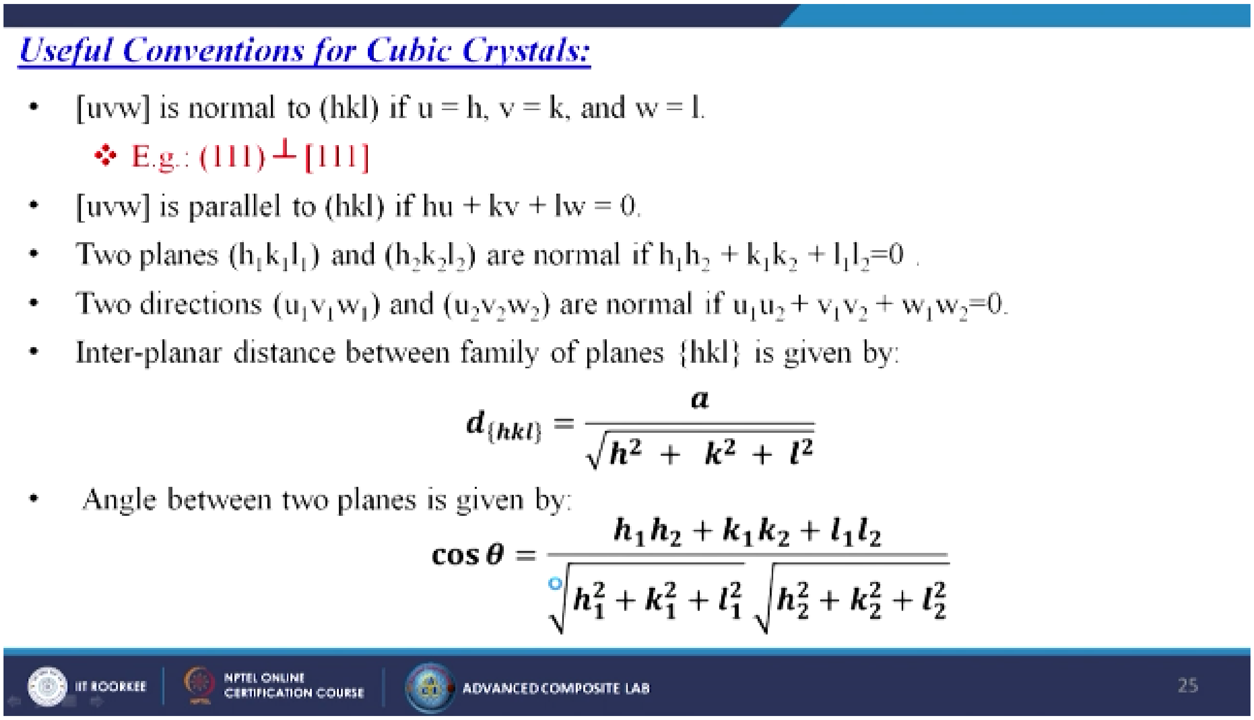
Miller Indices - Useful Conventions:

- If a plane is parallel to an axis, its intercept is at infinity and its Miller index will be zero.
- Never alter negative numbers:
  - ❖ This implies symmetry that crystal may not have.
  - ❖ Use bar over the number to represent negative numbers.
- A plane or direction of family is not necessarily parallel to other planes or directions in the same family.
- The smaller the Miller index, more nearly parallel the plane to that axis, and vice versa.
- Multiplying or dividing a Miller index by constant has no effect on the orientation of the plane.
- When the integers used in the Miller indices contain more than one digit, the indices must be separated by commas like (3,10,13).

of plane is represented by second bracket that is HKL, Miller indices useful conventions. If a plane is parallel to an axis its intercept is at infinity and its Miller indices will be zero.

Never alter the negative numbers, this implies symmetry that crystal may not have or maybe use bar over the number to represent the negative numbers if it is -1, so generally we are giving it as a 1 bar.

So a plane or direction of family is not necessarily parallel to other planes or directions in the same family, the smaller the Miller index more nearly parallel to the plane to that axis and the vice-versa. Multiplying or dividing a Miller index by constant has no effect on the orientations of the plane itself. When the integers used in the Miller indices contains more than 1 digit the indices must be separated by commas like 3, 10, 13.



Useful Conventions for Cubic Crystals:

- [uvw] is normal to (hkl) if u = h, v = k, and w = l.
  - E.g.: (111) ⊥ [111]
- [uvw] is parallel to (hkl) if hu + kv + lw = 0.
- Two planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$ are normal if $h_1h_2 + k_1k_2 + l_1l_2=0$.
- Two directions $(u_1v_1w_1)$ and $(u_2v_2w_2)$ are normal if $u_1u_2 + v_1v_2 + w_1w_2=0$.
- Inter-planar distance between family of planes {hkl} is given by:

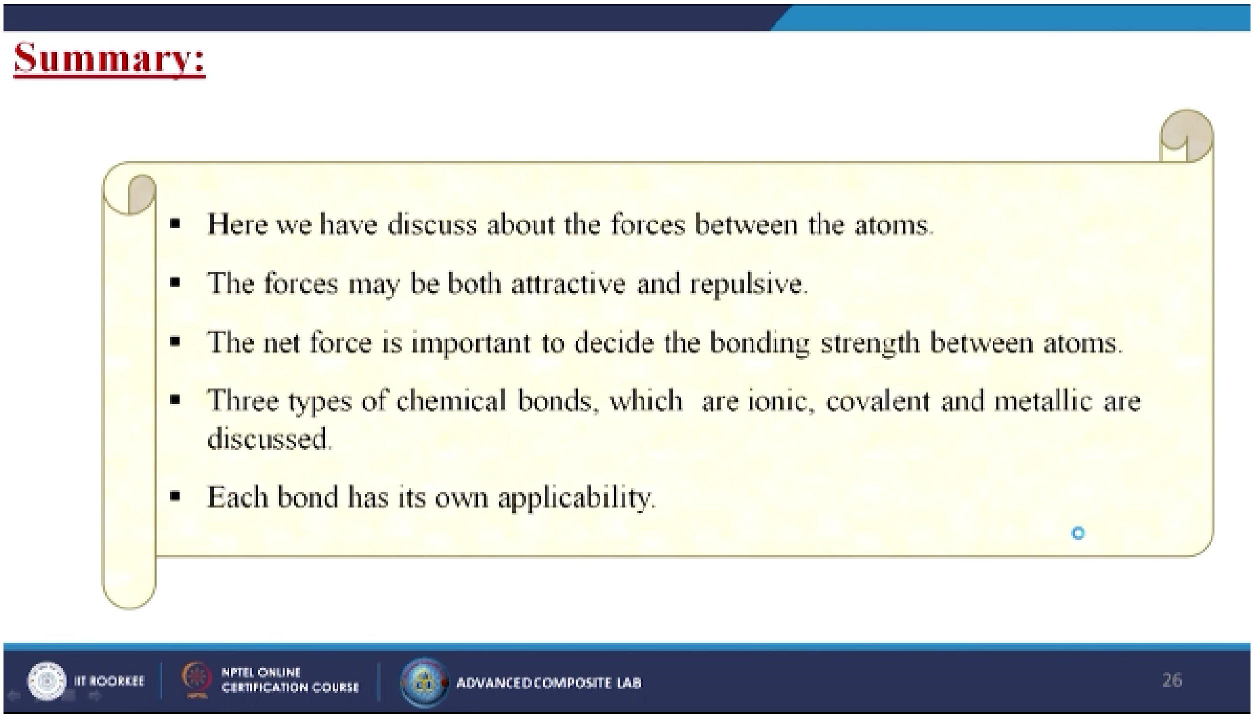
$$d_{\{hkl\}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

- Angle between two planes is given by:

$$\cos\theta = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{h_1^2 + k_1^2 + l_1^2}\,\sqrt{h_2^2 + k_2^2 + l_2^2}}$$

Now some useful conventions for the cubic crystals, so UVW within the third bracket is normal to HKL, is U = H, V = K, and W = L, example 1 1 1 perpendicular to 1 1 1, so here UVW is parallel to HKL if HU + KV + LW = 0, two planes H1, K1, L1 and H2, K2, L2 are normal like H1 H2, K1 K2 + L1 L2 = 0, two directions U1 V1 W1 and U2 V2 W2 are normal if U1 U2 + V1 V2 + W1 W2 will be 0, inter-planar distance between family of planes HKL is given by D HKL = A/root over A square + K square + L square, so this is the known formula. Angle between two planes is given by cos theta = H1 H2 + K1 K2 + L1 L2/root over H1 square + K1 square + L1 square into root over H2 square + K2 square + L2 square.

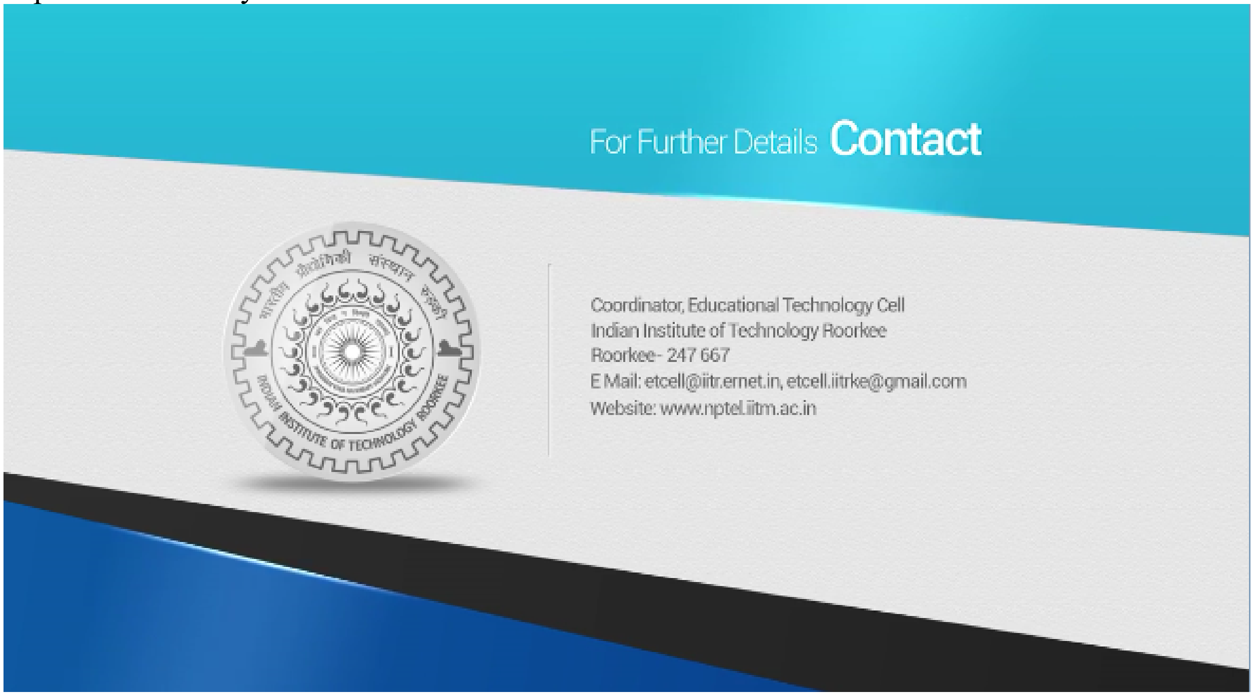
So now we have come to the last of this particular lecture so it's the time to summary or maybe the summarize the whole lecture, here mainly we are discussed about the forces between the atoms, different types of forces we have like some hydrogen then Van der Waals forces and



Summary:

- Here we have discuss about the forces between the atoms.
- The forces may be both attractive and repulsive.
- The net force is important to decide the bonding strength between atoms.
- Three types of chemical bonds, which are ionic, covalent and metallic are discussed.
- Each bond has its own applicability.

some kind of forces we have used, the forces maybe both attractive or maybe the repulsive in nature, the net force is important to decide the bonding strength in between the atoms, here three types of chemical bonds generally ionic bonds, covalent bonds, and metallic bonds we have discussed elaborately and each bond is having their own applicability based on that the material crystal structure or maybe the material physical properties or chemical properties is totally dependent. Thank you.



For Further Details **Contact**

Coordinator, Educational Technology Cell
Indian Institute of Technology Roorkee
Roorkee- 247 667
E Mail: etcell@iitr.ernet.in, etcell.iitrke@gmail.com
Website: www.nptel.iitm.ac.in

For Further Details Contact

Coordinator Educational Technology Cell

Indian Institute of Technology Roorkee
Roorkee-247 667
E Mail:- etcell@iitr.ernet.in, etcell@iitrke@gmail.com
Website:- www.nptel.iitm.ac.in

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Prof. Ajit Kumar Chaturvedi
Director, IIT Roorkee
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Dr. Kaushik Pal
Department of Mechanical and Industrial Engineering
IIT Roorkee
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Mohan Raj. S
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