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Lecture - 27 Introduction to crystals and bonding in crystals

We have been studying in the earlier lectures, how conductivity occurs inside materials, inside metal specifically. And there we consider how the electron moves through the solid, and we introduce different models to understand the motion of the electron through the solid. And we came became familiar with properties like electrical conductivity, the specific heat, the thermal conductivity, and even them some basic understanding of the magnetic properties of the material.

But while studying these different models like the Drude model or its more improved Sommerfields model we came across limitations. And these limitations showed us that considering the electron as a completely free particle moving inside the crystal is not the complete picture, it does not give us an accurate description of the electron moving inside the crystal.

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As you know that the crystal has an ionic lattice, which is a periodic arrangement of ions. And in our model the electron is considered to move freely as a plane wave through this crystal. And we have neglected all interactions of the electron with the periodic arrangement of ions. After all these are positive ions and they are periodically placed. So, the electron should feel a periodic potential because of this positive ions an attractive potential.

However, we have neglected all of these attractive potentials, which are coming from the periodic arrangement of ions. And this turns out to be one of the drawbacks of the Sommerfields model. And therefore, it cannot explain certain properties of the materials, which we will include now as we go along. So, certainly there is a periodic arrangement of ions which we cannot neglect. And there is a crystal structure a very periodic arrangement of these atoms inside the solid.

And this is nothing else, but leads us to the next topic, which is understanding the crystal structure. Because solid state physics to a large extent deals with studying behaviour of electrons and properties of solids, which have a periodic arrangement of atoms, ions or molecules inside, these structures. And so understanding a crystal structure is very important and that is going to be our next topic of investigation.

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So, we try and study the crystal structure of solids. Now, before we get into crystal structure what how does this crystal structure come about. The crystal structure comes about, because of atoms or different atoms coming together and forming bonds. And a periodic arrangement of these atoms results in the formation of a crystal structure. And

there are different types of bonds, which exist between the atoms forming the crystal structure. While I will not get into discussing the different types and the details of the bonds, I would just like to tell you what are the different types of bonds.

So, the different types of bonds are ionic bond. And a typical example of this is the sodium chloride crystal. Here what happens is that you have a sodium atom from which one electron is given out, which is accepted by chlorine. So, sodium forms a positive ion chlorine forms a negative ion, they get attracted to each other. And there is a periodic arrangement of this sodium chloride molecule across the system. So, this is called as an ionic bond, where there is the formation of these ions one of them donates an electron the other accepts an electron resulting in the formation of ions, which then attract each other. So, there are certain class of materials, which form these ionic bonds and the crystals which form out of them have ionic bonds inside them.

The second and very popular and well known class of bond is the covalent bond, this is where two atoms share electrons equally between them. So, two atoms for example, two hydrogen atoms can come together, you know of the hydrogen atom case. And the electrons from one hydrogen atom and the other hydrogen atom are shared between the two electrons and the electrons are shared between both the atoms.

And this leads to the hydrogen molecule, similarly there are solids in which there are covalent bonds very strong covalent bonds exist. And again in those atoms you have the items, which are equally sharing the electrons between them. The two atoms are approximately, the same electronegativity, have approximately the same electronegativity ok. Typical example which you will study later is a gallium arsenide system, where you have gallium and arsenic and the electrons are shared between these two atoms to form a covalent bond. And this system of gallium arsenide is repeated in space and you form a crystal, which is associated with gallium arsenide another example of covalently bonded system is the diamond.

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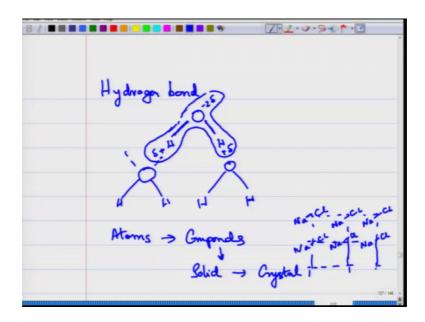
A crystal of diamond where there are carbon atoms, which are covalently bonded to each other to form the diamond structure and we will study that as we go along. So, you have the covalent a very well known form of bond, which is the covalent bond then you have the third which is the metallic bond. In the metallic bond you have as I have already told you that it is metals a large number of metals form this metallic bonds.

You have the ions which ionic cores, these are ionic cores and the outer most electron of these ionic of these atoms are and the electrons are delocalised they are delocalised over the entire crystal. So, these are delocalized electrons, which are not sitting on any particular atom, but the outermost electron has is completely delocalised and from a given atom, it goes around the entire crystal. And it gives rise to a sort of a glue which holds the positive ions together. So, the negative electrons there is a c of negative electrons all around between the positive ions, and these negative electrons acts like a glue to keep the positive ions in place, and this is the metallic bond ok. So, all your metals like copper and so on, these have metallic bonds inside them.

The fourth is called the molecular bond. Here the molecules or the compounds which make up the solid have dipoles inside them. So, the molecules have positive and negative ends inside them as a result of which there is an attractive. So, there is no exchange of electrons or sharing of electrons which goes on is just that the molecules are distorted, and they have positive and negative ends associated with them. So, there are dipoles.

And because of the dipole-dipole interaction, these molecules arrange themselves into an ordered structure, and there is an attraction between these molecules giving rise to the molecular bond ok. And for example, gases which are formed out of noble gases or solids formed out of noble gases or wax for example, polymers like wax and so on these have molecular bonds inside them.

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And finally, you have something called as the hydrogen bond; this is also very well seen in nature that you have a hydrogen atom for example, water. So, you have an oxygen atom and you have two hydrogen atoms. And there is a bond which is present between the oxygen atom sharing electrons with the hydrogen atoms. So, there is this covalent bond which is present between the oxygen atom and the hydrogen atom.

But what happens in this hydrogen bond is that the electrons are more displaced towards, the oxygen. They are more displaced towards the oxygen and so the oxygen has a slight negative charge and these gain a slight positive charge, because the electrons in these bonds are the cloud the electron cloud is a little bit more localised towards oxygen rather than the hydrogen atoms.

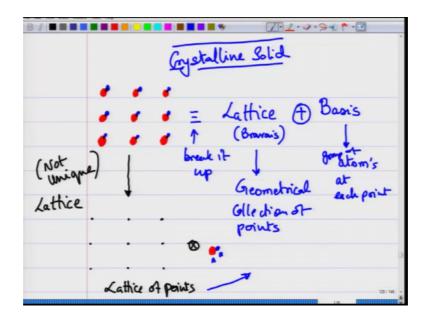
So, the electrons are almost stripped away from hydrogen and more localised near the oxygen, whereas the hydrogen remains like a naked positive charge and this positive end starts attracting the other negative ends of the molecule which can lead to so the electron cloud of an adjacent compound of this adjacent compound for example, another water

molecule gets attracted towards the hydrogen end, and this leads to the hydrogen bonding inside, and it can lead to a ordered structure. So, it can lead to an ordered structure of this water molecule, which can then organised itself into a lattice. And this type of hydrogen bonds is known in organic compounds and so on. It is very well known inorganic compounds.

So, by using these different types of hydrogen, different types of chemical bonds, you form a solid. So, from atoms you form compounds, which is two different atoms which will join together and form a compound. And from compound you form a solid, where these different components are periodically arranged in space to form a crystal. So, for example, sodium chloride, you can have this sodium chloride compound, which is sort of periodically arranged and you can form a crystal of sodium chloride. So, if this sodium chloride is periodically arranged in space, you form a crystal of sodium chloride. And so we will look at these crystals of sodium chloride and so on.

But this is the idea that you have atoms which are bounded to together, and then these compounds and these complexes or this collection of atoms are organised periodically in space leading to the formation of a crystalline structure. Where these are and there could be bonds between them, and you know these are the different types of bonds that exist, resulting in a periodic structure of this material. So, a typical sort of crystal will have atoms which are sort of organise.

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So, for one example you can have a red atom and you can have a blue atom, which are sort of periodically organised. I am just showing it to you in two dimensions. So, this is an example and you can keep on building this up. You can keep on making this bigger and bigger, I am just showing you a small part of it, but you can take these two atoms a red and a blue atom. And you can have even more complex shapes, and keep on replicating in space to form a crystal of this collection of atoms. So, this is a crystal, this is what we call as a crystal of where you have this combination of atoms, which are periodically repeating in space. And this combination of atoms as you move from this point to this point to this point, and you keep on going this combination of atoms remains identical.

So, now we would like to understand how to handle this sort of a crystalline solid. This is just one example. You can have examples, where there will be many more atoms which is a complex collection of atoms, but which have a periodic arrangement. So, whatever maybe 5, 6 atoms that same 5, 6 atoms in the same configuration are present here same configuration and they will periodically repeat them through space. So, to understand and to mathematically analyse these sort of crystal structures, we actually do an abstraction, we break it up this sort of a crystal solid, we break it up into a lattice plus a basis.

So, this collection of atoms which are periodically arranged in space, we can first break it up into a geometrical structure into a geometrical collection of points, and a basis is group of atoms at each point. So, what is the lattice corresponding to this collection of atoms, which are sort of periodically arranged. One way to define the lattice which is a geometric collection of points associated with this periodic arrangement of atoms in space. One way to define the lattice is say let us take a point here. Let us take the geometrical point which is sitting here, this is one way of defining the lattice point.

So, for this collection of atoms, I can consider the geometrical arrangement of points as just the points which are sitting between these two atoms. And of course, I have drawn a finite lattice this is an infinite collection of similar set of atoms distributed identically through space periodically arranged. So, I can from this complex arrangement of atoms in space, I can build up a lattice. Of course, by this particular way of going from this collection of atoms to the lattice is by no means a unique, it is not a unique choice, it is not unique.

But suppose I choose this procedure, and I get to this collection of geometric points, then my actual crystal is nothing else but this lattice of points where I will say that on each of these lattice points, I will put a configuration of atoms as shown here, where on each of these points I will put a red atom A and a blue atom B. So, I will take this lattice points. And on each of them if I start putting these collection of atoms AB on each of these points then I will land up with my crystalline solid.

So, this gives us the first conceptual understanding of how to handle a crystalline solid. And what is the lattice, which is associated with that solid the lattice, which I have drawn here is not atoms this is just a geometric set of points used to represent this collection of atoms which is present in the solid. So, it is just the collection of points used to represent this configuration, and on each point I am going to put this atom.