Introduction to Solid State Physics
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Lecture - 33
Indexing Crystal planes

In the last lecture we saw that we can have a variety of different crystal types or crystal lattice types and they have different properties; the Bcc lattice, the FCC lattice, you have the zinc blend structure, the diamond lattice and so on and so forth. And we classified and different materials can be put into these different type lattice types. Now, why is it important to analyze these different lattice types as you will see later on.

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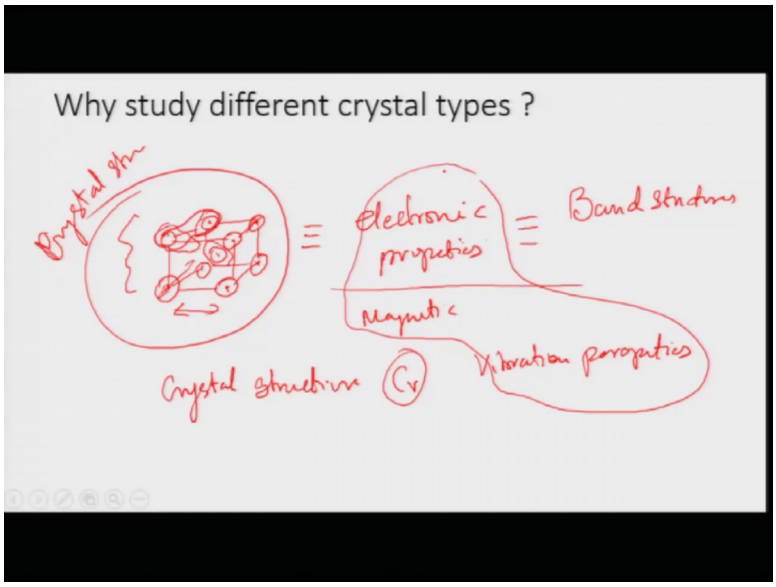

Depending on the nature of the lattice type if you have atoms which are arranged on a cubic lattice, then depending on the type of lattice that you have you can have one big atom in the centre,.

And the electrons in these items could be delocalized ok. The electrons in the atoms are not always around the ions which are present or the positive ion core which is present. Sometimes if you have an F-shell electron, they could be delocalized, they could be wondering much further than the nucleus, ok. Far away they can move to distances much far away from the nucleus the d shell electrons and so on and depending on the lattice

structure, you can have overlapping of orbitals along certain particular directions in the crystalline structure.

So, along certain directions the overlap might be strong and along certain other directions, the overlap might not be strong. That will immediately effect the electronic properties of the material. So, they have an immediate effect on something called as the band structure of the material. So, depending on the crystal structure and how the electrons are overlapping and delocalized along the lattice, you can have different types of behaviors of the bands inside the solid which are governed ultimately by the nature of the crystal structure. Depending on the crystal structure, the overlap of the electrons along some directions might be much more than compared to other directions.

Similarly, depending on the crystal structure, so this will effect electronic properties. Crystal structures immediately have a role to play on the electronic properties. The electronic property could become highly anisotropic. Along some direction there is more overlap, some directions there is no overlap at all or partial overlap.

It can effect this itself can effect magnetic properties because depending on the overlap of the wave functions with spins you can have ferromagnetic, you can have exchange interaction something called as an exchange interaction along some directions and not present along the other directions and so on. So, the symmetry of the crystal structure or the nature of the crystal lattice that is there governs the properties of those materials, the electrical property, the magnetic property. Similarly depending on the crystal structure certain types of vibrations are possible vibrations along certain directions are more probable than along different other directions. For example, vibration along the diagonal might not be so pronounced.

But vibration along these might become more pronounced in certain types of crystals. It varies from crystal to crystal even cannot generalize, but the crystal structure actually makes also the vibrations of these atoms very different and therefore, when you find the specific heat of the material, the specific heat of the material which has contributions of course from the electrons inside the material as well as contributions from the vibrating ions something which I have told you earlier, then the next specific heat of the material mostly the vibration of the ions actually is very different. The acoustic properties or the

vibration properties of the material depend on the nature of the crystal structure, what is the type of the crystal structure controls, all these different properties.

So, therefore what is the crystal structure is very important. It is an important ingredient which will go into understanding. Some of the properties which I have told you namely the electronic property, magnetic property, the vibrational property till now when we looked at the Druid's model, the Summer Fields model and when we looked at the electronic magnetic and vibration and the specific heat of the electron, we did not look at the vibrational properties

But we looked at least a specific heat of the electrons know where did we introduce anything about the shape of the lattice, but now as then that is why there were quite a few drawbacks. It could not explain many of the things, but now once you have a way to analyze the lattice and the tools that have been given to you to analyze the lattice, you can use it to understand how the electrical properties change and what new things start emerging to explain features, which were not explained in the earlier theories because they did not take into account a presence of an underlying lattice which has a particular very definite structure and electrons are interacting with that structure in the lattice. So, it is indeed very important to define and understand the crystal types and study their properties.

Now, another very important thing another important tool till now we have been using various tools to analyze the crystal structure, namely the primitive lattice, the primitive lattice vectors, the primitive cell, the primitive volume, the unit cell, the conventional unit cell, all are these are tools, the symmetry properties, all these are tools to understand the lattice structure along with them.

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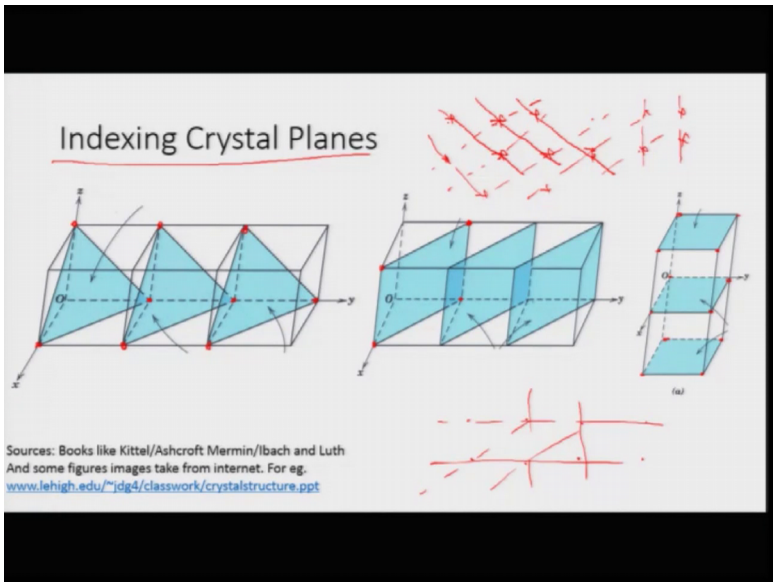

You have one can ask another question that if you have a lattice of points, a lattice of points it is a simple lattice in two dimensions. I can define different planes of atoms ok, I can define a plane of atoms and these planes are all parallel to each other. One plane of atoms that I can define is like this and I can go on, ok. I can define planes of atoms or I can define another plane which is along this direction ok, I can define planes of atoms which are along other directions and so, I can define many different types of planes.

I can define this vertical planes where I will have lattice points sitting on those planes. So, inside a lattice I can define many different planes on which I will have lattice points which are sitting is there a way to classify and categorize different types of planes in the lattice and that brings us to the topic of Indexing Crystal Planes.

So, in a three dimension I showed you in a two dimension there are different types of lattice planes. I can define some verticals you can define horizontal lattice planes. If I have this set of points of course then you can define horizontal lattice planes, vertical lattice planes, I can define those at an angle and each of them will contain lattice points or atoms on them. Three dimensional lattice crystal planes will have you can have these parallel set of planes which will contain lattice points. These are for example.

In a cube you can see these points which are at the corners of the cube and for this blue color lattice plane you have these three points which has sitting on them and similarly, I can define a parallel set of points for this plane which is along this direction. I can define

an another plane where I have these four points which are sitting along this plane and similarly, there are parallel set of planes. I can have another set of planes which are like this. What distinguishes these different planes what is the way that I can identify and each of these planes actually collects a certain set of atoms.

Along certain direction, these planes are oriented along certain directions is there a way to classify these different planes namely if I give you a certain number or if I give you a certain quantity, then I can immediately say that I am not talking of each of these plains, but I am talking of all these planes,.

So, just with one particular combination of numbers, is it possible to define certain types of planes and therefore, come up with a way to define any type of planes in the system and whatever we will we will do, we will not do an indexing for this plane for this plane, for this plane, but if I come up with the scheme of indexing, it will define all the planes which are parallel to each other for whatever indexing, I do for this plane will be the same for all of these planes. Whatever indexing is for this plane, it will be the same for this, similarly for this and this procedure of classifying planes is called the Miller's Indices and it will become very useful as we go along for classifying lattice planes and planes of atoms inside a solid.

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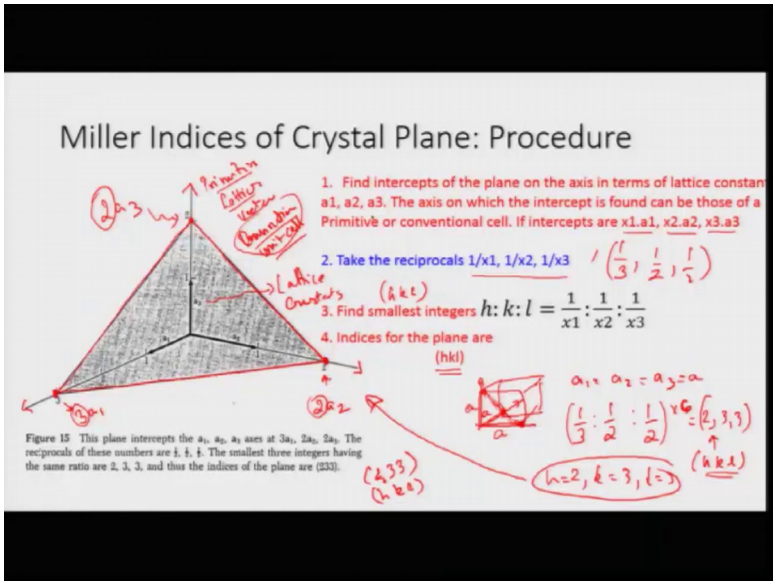

So, for now I will just give you what is the procedure for finding a Miller Indices associated with a plane. So, suppose you have a crystal, this is the lattice plane of a cubic

crystal, but suppose the crystal is not cubic, it is distorted, then you have three directions with the fundamental lattice constants which are a 1 a 2 a 3 in a cubic crystal. The lattice constants are all a if you recall for a cubic crystal, the lattice constants are all a, but if I distort the crystal along the three directions, then I can in general talk of a 1 a 2 a 3 and let us talk of a lattice plane which is this lattice plane of atoms which is shown here as this plane which is sitting inside the structure.

If a 1 equal to a 2 equal to 3 if a 1 equal to a 2 equal to a 3, then of course I have a cube, then this is a cube and these points are sitting at this three corners of the cube and this is the lattice plane.

But in general I am taking that a1 is not equal to a2 not equal to a3, then how do I define, how do I index this plane? What you first do is that find out the intercepts along the axis. These axis can be the primitive axis or the axis of the conventional unit cell. So, I first find out the intercepts of this plane along the three axis of the system and these axis could be either primitive lattice vectors or vectors along your unit conventional unit cell.

There is no restriction conventional unit cell, but whatever you define you have to stick to it, ok. So, for the cubic cell of course it is very easy you are primitive unit cell and the normal ones your conventional and the primitive are both identical. So, along these three axis which are the fundamental translation vectors of your lattice, it could be either primitive and non-primitive namely along the conventional unit cell you find the intercepts. So, a1 and you write it in terms of the lattice constants, these are the lattice constants.

So, if the intercepts are x 1 a 1 x 2 a 2 and x 3 a 3 ok, these are the intercepts. For example, in this example this intercept is 3 of a1, this intercept is twice of a 2 and this intercept is twice of a 3 ok. So, I first find the intercepts, then I take these values and I take their inverse, ok. I take the inverse of the intercepts which are written in terms of the lattice constants after I take their inverse, then find out 1 by x 1, 1 by x 2 1 by x 3. So, I find out 1 by 3, 1 by 2, 1 by 2.

These are the inverse of the intercepts, then I have to find out what is the smallest integers hkl, the smallest set of integers hkl whose ratios are exactly identical to the ratios of these intercepts. So, I have to find out the ratios of the intercepts inverse of the intercepts. What I do is that, I can multiply it by the least common factor for them and I

will get intercepts 2 3 3. These are my hkl. So, if I get do this procedure, then I will find out a unique index which is indexed by this collection of hkl integers. The hkl integers h is equal to 2, k is equal to 3 and l is equal to 3. In this particular example these index not only this plane, but all the plane which are parallel to this plane, all the planes in the lattice which are parallel to this plane are all indexed by this unique number 2 3 3 hkl and these hkl are called Miller Indices and this gives a way to index different lattice planes along different directions in the crystal.

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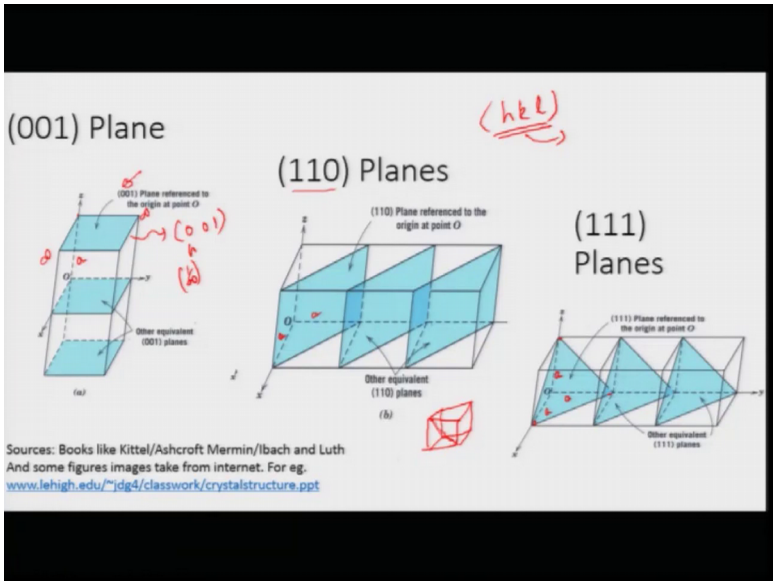

For example, if you have this lattice plane shown here, it has an intercept along a. If a is the intercept along this direction, it is a cube ok, but the intercepts which are along the x and y are infinity and along the y direction are infinity. So, intercepts of this plane along the x and y are infinity, but along the z direction it is finite. So, the Miller Indices for this plane is 0 0 1, you remove the comma. The Miller Indices h is equal to this is of course 1 over infinity, it will give 0 0 and 1. So, this is taken as the 0 0 1 plane defines all the planes which are cutting the z axis and parallel to the xy plane in the cube 1 0 9 is of course this plane it has no intercept along the z axis, but intercepts of a and a along this.

So, this is 1 1 0 plane and similarly the 1 1 1 plane is for a simple cube there 3 intercepts and this is your 1 1 1 plane which is going along the diagonal of the cube. So, if you have a cube and a plane which is along the diagonal of the cube, ok.

So, you have a plane which goes along the diagonal of the cube, then that is your 1 1 1 plane which you can define and with this you can identify different set of lattice planes and index them. You do not have to write an index or when you want to talk of a lattice plane, you do not talk of this individually, this individually, this individually, but you talk of an hkl lattice plane which immediately specifies what is the orientation and direction of that lattice plane.

So, this becomes a way to actually analyze crystal structures and we will continue now to understand some of the properties of these crystals as the diffract light or electromagnetic waves and here use of these indices will become very essential which we will continue in the next few lectures.