Solid State Chemistry
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Lecture – 37
Miller Indices for Hexagonal System, Distance between Planes

Now, I will start the 2nd lecture of the 8th week of this course. In this lecture I will talk a little bit more about Miller planes we will take the special place case of the Hexagonal System and what is called the Miller Bravais indices. And I will also talk about this distance between Miller planes and this as you saw in the last lecture the Miller planes are Miller indices are used to represent these lattice planes ok.

We will restrict the discussion to Miller indices for lattice planes in this lecture we will not talk about Miller indices for directions ok. And what I want to show is just give you some more special cases of Miller indices that is Miller indices for the hexagonal system and also talk about the spacing between these lattice planes ok. So, week 8 lecture 2 will be Miller indices for the Hexagonal System and the distance between planes.

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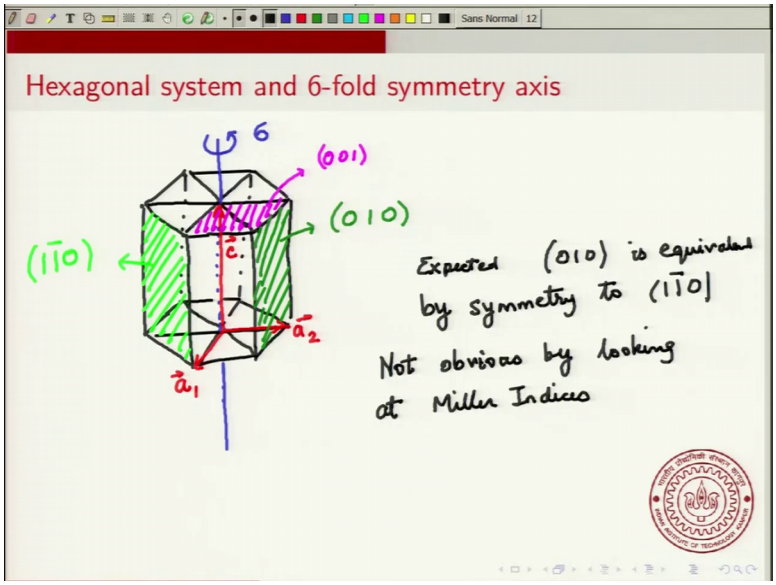

So, the hexagonal system has a 6 fold symmetry axis ok. So, if you look at any hexagonal system then you essentially have a 6 fold axis of rotation. So, it is characterized by this 6 fold axis of rotation I am just showing it in a; I am showing it in a

you know I mean this is to be treated as perpendicular to the plane of the screen. And you can imagine something else like this and you can plead this and this is the hexagonal system.

This is a typical hexagonal system and you can see that there is a 6 fold axis of symmetry you can I will show it by this color. So, this has a dotted line. So, now this is a 6 fold axis of rotation and in such a case ok; now if you take the; if you take the unit cell for this. So, the unit cell is typically taken as this. So, it will be taken as a 1, a 2 and c ok.

So, these are the Miller indices ok; I am using a 1 and a 2 instead of a and b and that will become clear why I am using a 1 and a 2. But you can also think of it as a b and c and this these are the primitive translation vectors for this cell or these are the vectors for the unit cell for the and this is usually chosen as the conventional tool itself for this system ok.

Now, in this case if we look at; if you look at let us say we look at this plane ok. Now the Miller in this index for this plane is 0 1 0 ok; now let me look at the Miller index for this plane ok. Now this plane has the Miller index. So, it intersects the a 1 axis at 1; so, it is Miller index for the a 1 direction is just 1. The a 2 axis it intersects at minus 1; so it is 1, 1 bar and it does not intersect the c axis; so it is 0. And let me take one more plane just for completeness; let me take; let me take this plane. This plane is clearly this 0 0 1 ok; now one of the; one of the things that now the hexagonal system has a 6 fold axis of symmetry.

Therefore, we expect 0 1 0 surface should be equivalent by symmetry is; let me write it down explicitly is equivalent by symmetry to 1 1 bar 0. And now in the case of the cubic system we saw how equivalent directions were related by just a permutation of the indices ok. But here these two do not have any the equivalence between these two is not obvious; if you look at the indices ok. It is clearly we see that these indices are it is not; this is not obvious looking at Miller indices ok.

So, if you look at 0 1 0 and 1 1 bar 0 for a; now they are actually equivalent by symmetry, but that is not obvious when you look at the Miller indices and this is the problem that is addressed by the use of what is called the Miller Bravais indices.

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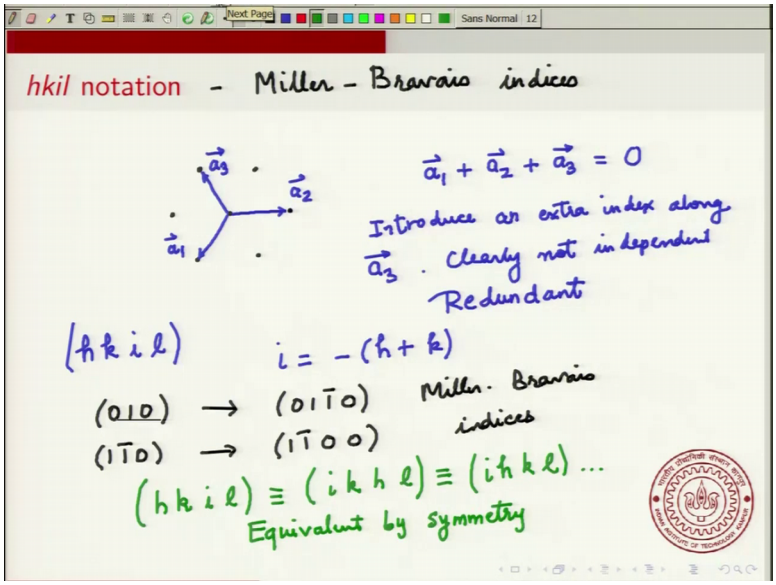

And this is the hkil notation this is also known as the Miller Bravais indices ok. So, instead of just calling it the Miller indices sometimes it is called the Miller Bravais indices ok.

So, the basic idea is the following that if I let me just look let me assume that the screen is perpendicular to the c plane and so this hexagonal system will look like a perfect hexagon here ok. I am just showing; I am just showing the and we had the lattice translation vectors a 1 and a 2; c is perpendicular to the screen and I am not showing it.

Now, if I imagine taking third a 3 ok; then if I can see that a 1 plus a 2 plus a 3 is equal to 0. So, they clearly add up to 0 ok. So, now the idea of this Miller Bravais indices is to introduce an extra index along a 3 ok. So, just as you had Miller index along a 1 and a 2; now we introduce an extra Miller index along a 3 ok.

Now, clearly this is not independent ok; in fact, it is called redundant; redundant means it is not really needed it is an extra index which is not necessary to describe the plane ok; however, it is usually still useful. So, we use a notation h k i l and because of this relation we have i is equal to minus h plus k ok. So, now how does this help ok? So, let us go back to what we had in the last slide.

So, we had the 0 1 0 and the 1 1 bar 0 ok. So, now the 0 1 0 goes to 0 1 1 bar i is equal to; i is equal to minus h plus k; now h; h is 0, k is 1. So, a minus of h plus k is minus 1;

so 0 1 1 bar 0 ok; so that is 1 bar. Then the next case we had 1 1 bar 0 and in this case; in this case i is equal to minus of h plus k; h plus k is 0. So, i is equal to 0; so it has 1 1 bar 0 0 ok.

And so the Miller Bravais indices ok; so you see this Miller Bravais indices are actually 4 indices instead of 3 ok. The 4th one is reserved for the c axis of and the other three are reserved for a 1, a 2 and a 3. And you can see that is that these two equivalent directions they are represented by a permutation of these numbers ok. So, you can permute these index indices between each other and you will still get equivalent directions.

So, in other words; in other words h k i l is equivalent to i k h l which is also equivalent to i h k l and so on ok. So, you can take; you can take up to up to you can do the 6 permutations of these and you will get equivalent directions; so these are equivalent by symmetry ok. And what we see is that introducing this what we see is that introducing this redundant index allows you to immediately identify equivalent directions ok. So, this is called the Miller Bravais indices and this is very commonly used for hexagonal systems ok.

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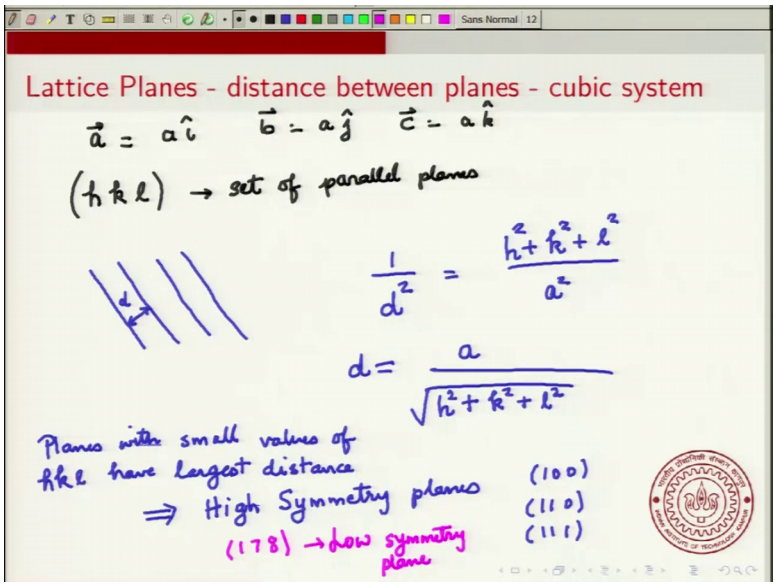

Now, next let us look at these family of lattice planes and look at let us ask what is the distance between lattice planes? First let us consider a cubic system, so in a cubic system the cubic system you have a is equal to ai, b is equal to aj, c is equal to a k. So, these are

the three primitive translation vectors they are all they all have the same length and they just point in different directions; they have their point in perpendicular directions.

So, now if you have Miller index h, if you have a; if you have a family of planes given by hk l. So, this is a set of parallel planes then you can ask what is the distance between these planes if you have; if you have let us say one plane, then you can ask what is the distance what is the perpendicular distance between these two planes ok. And this turns out to be a fairly important quantity and I am not; I am not going to do the derivation of this ok; it is fairly simple geometry, but in the case of; in the case of cubic ok, you can just show that it is equal to you can write this relation 1 over d square d is distance between the planes is equal to h square plus k square plus l square divided by a square ok.

In other words d is equal to a divided by square root of h square plus k square plus l square. So, that is the distance between these set of parallel planes ok; again I am not going to do this derivation**.** So basically if you had a plane; so what it means is that planes with small values of h k l have largest distance ok. So, they are the ones that are that have the largest distance between them and these are also referred to as high symmetry planes ok.

So, those planes that have small values of hkl, they are referred to as high symmetry planes and they have the largest inter planar distance ok. So, if you give Miller index like ah; so 1 0 0 1 1 1 1 0 1 1 1; these are all the high symmetry planes. And if you have; if you have something like you know so on the other hand if you have something like let us say 1 7 8 ok; this is not a high symmetry plane; this is a low symmetry plane ok.

And the reason this is called these are called high symmetry planes and low symmetry planes is that if you look at; if you look at that plane you will see that in that plane there are some of these symmetry elements, which are there in the overall crystal ok. I will not discuss too much in detail about that, but basically you keep in mind that small values of h k l they have the largest distance and these are referred to as high symmetry planes ok.

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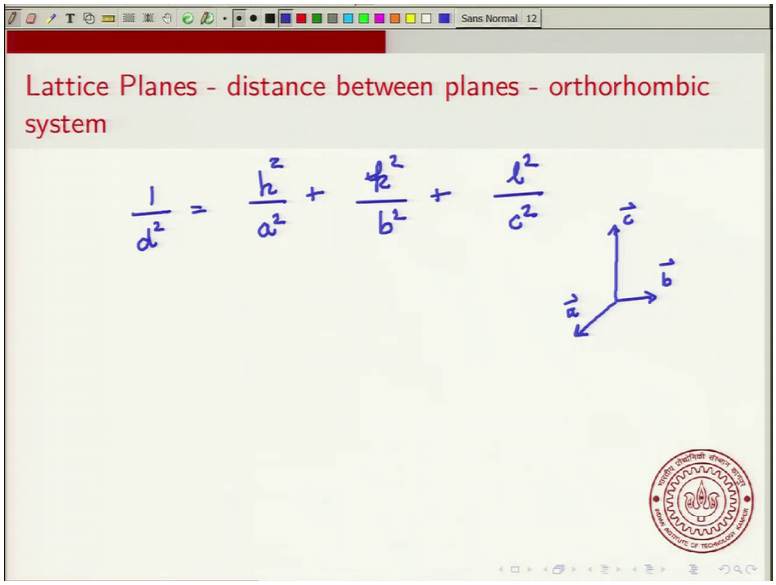

Now, what about the case when you have let us; when you have let us say an orthorhombic system? Now in this case the formula just changes a little bit. So, 1 over d square is equal to h square over a square plus k square over b square plus l square over c square and this is another no very well use formula ok.

Now, notice that again you have abc perpendicular to each other ok. So, you are; so you can just use something like a Pythagoras rule ok. So, they are all perpendicular to each other only their lengths are different and in this case you can calculate the distance using this formula ok.

Now, so far so good and you know it is these formulae are fairly easy to derive at least at least for cubic and orthorhombic systems ok. But we can also derive them for the more general case and but in that case the expression becomes fairly complicated ok. So, let me just write the general expression ok; I will not; I will not expect you to derive it or remember it.

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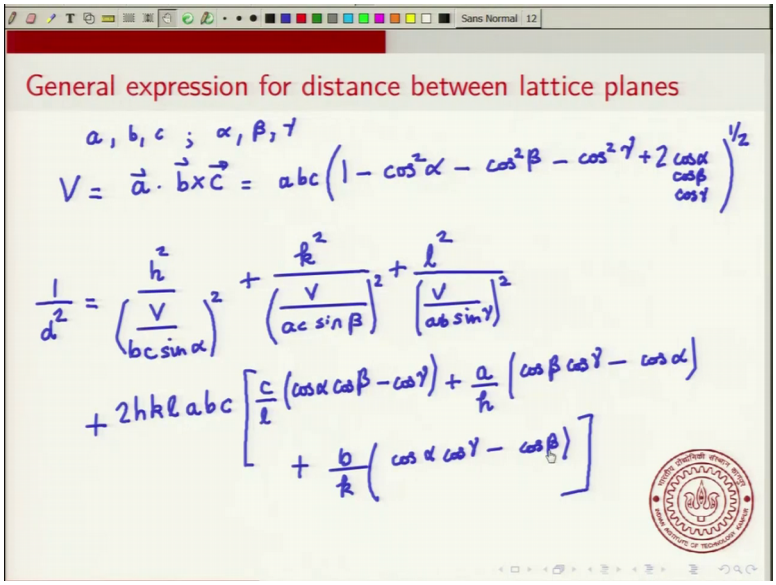

But basically the general expression for distance between lattice planes, now, you have a, b, c, alpha, beta, gamma. So, you could have all these and the general expression in order to write the general expression ok; we first write the volume of the unit cell ok.

Now this as we said it is given by a dot b cross c the scalar triple product and this can be written as abc 1 minus cos square alpha minus cos square beta minus cos square gamma plus 2 cos alpha, cos beta, cos gamma. So, it is a product of all these and this whole thing raised to half ok.

So, this is cos alpha cos beta cross; so here what I mean is a product of all these cos alpha into cos beta into cos gamma ok. So, it is this whole thing raised to half. And so, this is the volume of the cell of the unit cell formed by these three primitive translation vectors and or these three lattice translation vectors.

And now the distance between planes between hkl planes can be written in the following way h square divided by V by bc sin alpha plus k square divided by V over ac sin beta square plus l square divided by V over a b sin gamma square plus 2 h k l abc. And you have c by l cos alpha cos beta minus cos gamma plus a by h cos beta cos gamma minus cos alpha and you can see; you can see that there is a symmetry in each of the terms b by k cos alpha cos gamma minus cos beta ok.

So, as I actually you can see that you have one type of term which curl which comes from this h square divided by V by bc sin alpha; for and then once you have this you can just switch h to k switch b and c to a and c and alpha to beta and you will get this. And similarly again by switching things you can get this and then you have this additional term this is h kl into abc and you have this expression, but again each of these expressions is this it looks very similar ok.

For example you have a by h cos beta cos gamma minus cos alpha. So, similarly here b by k cos alpha cos gamma minus cos beta; so this is the general expression for distance between lattice planes. And this expression even though it looks a little big it is extremely useful and this is probably the I mean the fact that you can write such a general expression allows you to index X ray diffraction patterns ok; that tells you about it gives a lot of information about the structure we will see this when we discuss; when we discuss X ray diffraction.

So, I will conclude this lecture here ok. So, here and with this I will conclude the discussions on Miller indices. We can see that these Miller we have seen the Miller indices for planes and so what we have seen is that Miller index is a very useful way to characterize planes and to characterize these lattice planes. And we can also calculate the distance between these lattice planes and it is this distance between lattice planes that will be probed by powder X ray diffraction and this will be the topic of the next few lectures.

Thank you.