Solid State Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture – 36
Miller Planes, Miller indices

Now, I will start the 8th week of this course. In this week and the following week, we will discuss about X-ray diffraction and the concepts related to X-ray diffraction in particular that of the Miller Indices. So, I will start with a discussion of Miller Indices ok.

So, in this first lecture of week 8, we will be talking about Miller Planes and Miller Indices.

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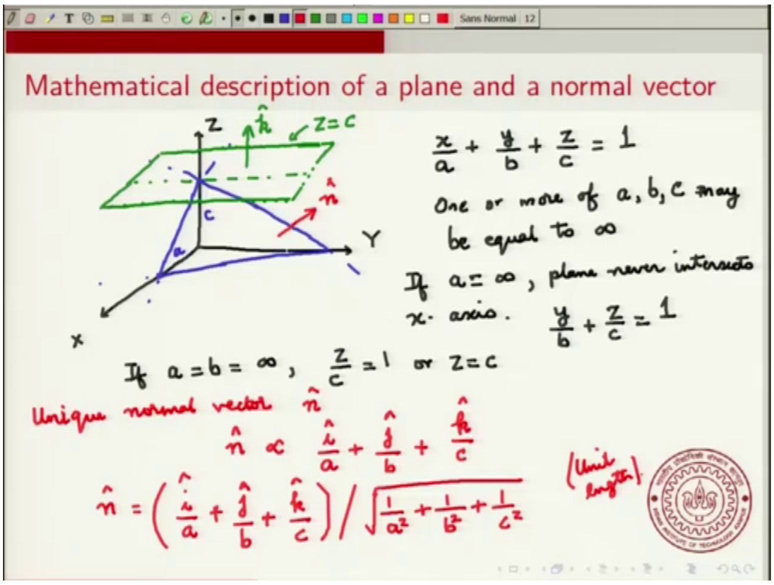

First, I will talk about the mathematical description of a plane and a normal vector. So, let us consider a general Cartesian coordinate system ok. So, you have X Y and Z axis. X, Y and Z axis ok. These are perpendicular to each other and in this case, if we had a plane ok, then the plane will intersect each of the axis at some point.

So, let us say it intersects the X axis at point at point a, the Y axis at point let me show it b, the Z axis at point c ok. And now, so this plane intersects each of these axis and this plane is a two-dimensional object that looks something like this ok. We write this c again; c is the intercept on the Y axis and a is intercept on the X axis ok.

So, now the plane formed by joining these three points ok, this plane will of course, it will it will it will extend in all directions ok. So, it is not it is not only limited to this triangular region, but it extends in all directions ok. So, this plane the equation of this plane is given by x divided by a plus y divided by b plus z divided by c equal to 1. So, this is the equation of the plane and many of you might be familiar with this equation of a plane.

So, you can write the plane equation in many different ways, but essentially it is convenient to write it in this form where you have x over something plus y over something plus z over something equal to 1 ok. Now sometimes, sometimes b or c might be sometimes one or more of a b c may be equal to infinity. So, for example, if a equal to infinity, if a equal to infinity; that means, the plane never intersects the x axis ok; that means, this plane never intersects the x axis ok.

So, it means never intersect x axis ok. And in this case, the equation will just look like y over b plus z over c equal to 1. So, the equation will simplify, there will be no x term ok. Now similarly you could have you could have 2 of, if a equal to b equal to infinity ok. Then the equation is z over c equal to 1 or z equal to c or z equal to c. And you can see this, so this plane now I will just show it in a different color. So, it will look like this; so it intersects the z axis at c and it is essentially parallel to the x y plane.

So, it intersects the z axis at z equal to c, but it is, but it is parallel to the x y plane ok. So, it never intersects the x or y axis ok. So, this basic description of a plane so, let me write. So, this is the z equal to c plane ok. So, you notice that I am describing the plane here using z equal to c instead of instead of saying z by c equal to 1, but that is the same.

So, essentially what I want to say is that this way of a describing planes is fairly useful ok. Now let us talk about a vector that is normal to the plane. So, for any plane you can draw a vector that is normal to it. So, this so, I want to consider a vector. You can draw it at any point in the plane ok. You can draw a vector that is normal to this plane; normal vector and usually we take it to be a unit vector.

So, so you can make a unit normal ok. And wherever you draw it, whichever point you draw on the plane it will be the same vector ok. So, there is a unique normal vector to every plate. So, I will just write it in red, there is a unique normal vector and this unique normal vector is n and it can be shown that again from basic geometry ok. You get the idea that the components of the normal vector. So, we can write n hat is proportional to I am writing proportional to ok, a vector that is given by i by a plus j by b plus k by c ok.

So, that is the normal vector ok. So, you can go back and ask you know suppose we consider the case where a and b are both equal to infinity. If a and b are both equal to infinity and z by c equal to 1, then the normal vector then in this first expression, a goes to infinity. so this goes to 0, b go b goes to infinity, so j by b goes to 0. So, you are left with just k by c ok.

So, the normal vector is proportional; that means, it is parallel to k by c. So, that is in the direction of z and you can see that that makes sense ok. So, you can see that for this the normal vector is in this direction ok. And actually, the unit normal vector is just k hat in this case ok. So, what you have to, I have said that it is proportional to this. If you want to find what it is equal to what is a constant of proportionality ok, then you can do that you can do that quite easily. You can just divide this by the normalization constant ok. So, it is by the length of this vector. So, we take this vector divide it by its length and you will get the constant of proportionality.

So, what is the length of this vector? The length of this vector is a square root of 1 over a square plus 1 over b square plus 1 over c square ok. So, n hat, I will just write the answer. So, this is equal to i by a plus j by b plus k by c divided by divided by square root of the length of the vector that is 1 over a square plus 1 over b square plus 1 over c square. So, this is the length of this vector ok.

So, if I take a vector and divide it by its length I will get a unit normal unit vector along that direction. So, this is the unit normal vector ok; so this has unit length. So, this resulting vector will have unit length. And I would not bother you know expanding on this expression, but here you get the idea of a plane and a normal vector ok.

Now, what we realize is that, this intercepts on the axis are very useful to describe planes and. So, we will be expanding on this use of intercepts in the, we will be using this to the concepts of lattice plates in crystals.

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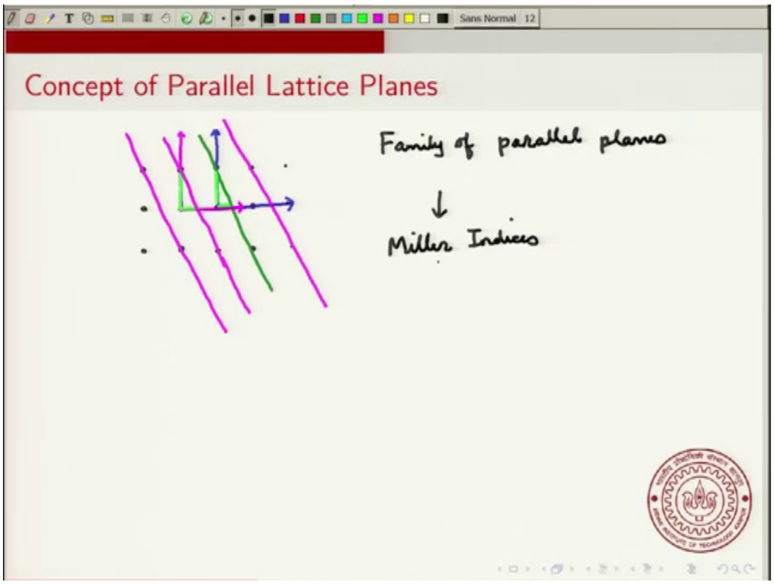

So, if you take a crystal ok. Now in this crystal, the first thing ok let me just again I will use 2 dimensions for illustrations ok. And so a plane will look like a line in this case.

So, let me just take a simple square lattice. Now let me, fix my origin say I will fix my coordinate system with my origin here ok. And now if I think of planes, if I think of a lattice plane, let me I will just take an example of a lattice plane. Did we put a few more points? Ok. Now you see this plane ok, so this is passing through these. This is passing through this atom and this atom ok.

Now, I and essentially if you look with this respect to these coordinates, it forms. It makes these intercepts, it makes this and this are the intercepts; intercepts on the two axis ok. Now the crystal has a translational symmetry, so I could take, I could imagine that I do the same thing now with at different origin. let us say I do it at this and let us say I do it using this point as the origin and let me take a different color and use let us say using this pointer, that is the origin ok.

And now if I do, if I take exactly the same intercepts that I took here, so I take this and this ok. Then my resulting lattice plane I will get a plane that looks like this. And as you can guess, it is parallel to this other plane it is parallel to the plane in green. So, the plane in plane in purple is parallel to the plane in green. And you can do this and you can get a series of parallel planes. You can get a series of parallel planes ok. And I will just, I will just show some other parallel planes.

So, for example, you will get something that looks like this. Something that looks like this and so on ok. And in some sense, these planes are all the same plane ok. These planes are all the same plane ok. Just they are just parallel to each other, but essentially that is the same because you just changed your origin from one place to another. But, essentially there is something because of the translational symmetry of the crystal, these planes are in fact identical ok.

And so, this is the so, we have this concept of parallel lattice planes ok. And sometimes, this is referred to as a family of parallel planes or just a set of parallel planes ok. And so now, we would like to have a notation to describe this family of lattice planes ok. And clearly, we will so, look for a general. So, and this notation will be called known as the Miller Indices ok.

So, this is used to describe this family of parallel planes and crystals ok. And we will just illustrate the use we will just the illustrate how the Miller Indices are calculated and it will become very clear.

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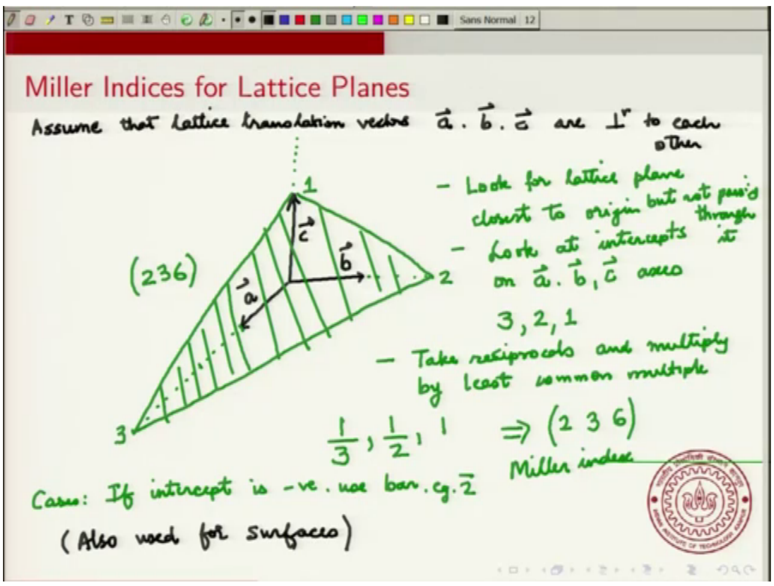

So, let us look at miller indices for lattice planes. So, here what is done is, you choose your crystallographic axis. So, let us so first we will assume that lattice translation vectors a b c are perpendicular to each other.

Now, I mean a actually it does not even matter we do not need to assume that, but let us just start with that ok. So, now, you will have your crystallographic axis. So,, let us say you have you have a you have b and you have c and these are all perpendicular to each other ok. Now what you do is, you have these parallel lattice planes and you will look lattice plane closest to origin ok.

So look for that lattice plane in that family of planes that is closest to the origin and let us say it. Now let me just draw that plane let us say this was my plane, let us say this green thing is the plane that I am considering ok. And now use you look at intercepts.

So, you look at the intercepts on the a, b and c axis ok. And what you see is that, the intercept on the a axis is at is at let me say this intercept is at is at 3, b axis is at 2 b, so it is two in fractional coordinates and this is at c, so it is 1. So, let me say that the inter just I am just taking an example where you have a plane where the intercepts are 3 that is 3 a on the a axis 2 or 2 b on the b axis and 1 c on this c axis ok.

Then take reciprocals and multiply by least common multiple, by least common multiple ok. So, what you will do? If you will take the reciprocal, so you have 1 by 3 1 by 2 and 1 ok and now I will multiply by the least common multiple. Least common multiple clearly is 6. So, you get 2 3 6 ok and this is the Miller Index.

So, the Miller index for this plane is 2 3 6 and you put it in a square bracket. There is no comma or anything ok. It is just written as 2 3 6 ok and you will use a you use a square bracket ok. So, so this is how the Miller Planes are you can you can calculate the Miller Index for a plane. Now some points to keep in mind ok, special so cases. If intercept is negative, intercept can be positive or negative, so it could intersect the axis on the negative side also; if you intercept is negative, use bar.

For example 2 bar etcetera ok; so that is one important thing ok. And intersect can be infinity ok, intercept cannot be 0 ok. So, if it is 0, then it will also intersect at 1. So, if it is 0, then there will be a parallel plane that into a intercept set 1; intersects at 1 ok. So, that that should be the one that is considered ok, the closest to the origin, so the plane should not pass through the origin ok, but not passing through it ok.

So, the so we look for the lattice plane that is closest to the origin, but not passing through it ok. So, then no intercept can be 0 because the lattice plane will not pass through the origin. If you get a lattice plane that is intersecting one of the axis at 0; that means, it will pass through the origin and that then you take the next lattice plane that is parallel to it, but not passing through the origin ok.

So, these are the Miller Indices for the lattice planes.

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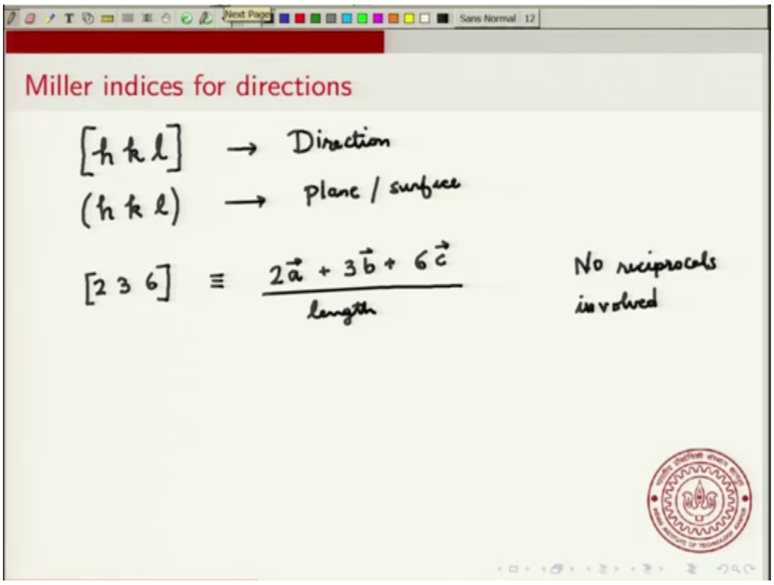

And now, we can also use Miller Indices for directions ok. And this, this is another very common thing that is used. So, here this is used for a lattice plane ok. You can also use the same for also used for surfaces. So, you can say, say the 2 3 6 surface. You can call this a 2 3 6 surface of this crystal ok; now we saw the concept of a normal vector ok.

Now, Miller Indices are also used for directions ok, but here the notation is so, you can say for example, you can talk about the crystallographic directions. You can talk about the a b c directions ok. So, in this case the notation is different. So, h k l, so h k l is the usual symbol used to describe the Miller Indices. And if you put it with a square brackets as opposed to round brackets, so this is represents a direction ok. Whereas, let me remind you again the h k l with the curly brackets represents to a plane or a surface.

Now, actually the way you construct. So, suppose I say, a direction of 2 3 6 ok, what would the direction be? So, a direction of 2 3 6 ok; so this corresponds to 2 a plus 3 b plus 6 c square root of 2 square plus 3 square. Well, we have taken a b and c perpendicular to each other to, so and divided by the length of this vector.

Let me I will just say, I will just say divided by length of the vector ok. So, the point is at 2 3 6, the direction of 2 3 6 is along this 2 a plus 3 b plus 6 c ok. There is no reciprocals; no reciprocals ok. So, when you are describing Miller Indices for directions, there are no reciprocals that are involved ok. So,, keep in mind that usually the round brackets is used for issues for planes, Miller Indices for planes or surfaces whereas, the square brackets is used for directions ok.

Now, there is one more now you can extend this for what I have been talking so far is you can use it for for cubic or non-cubic system ok. You can use it for any of the 7 crystal systems ok. And that is not a problem at all ok.

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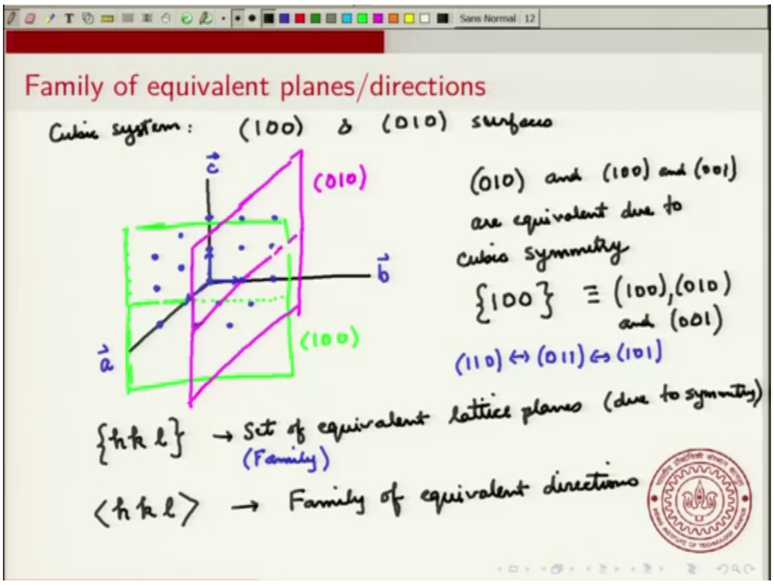

Now, let us consider the case of cubic ok; let us consider a cubic system ok and here, now if you consider the, the 100 surface and 010 surface ok.

Now, let me draw these surfaces, so ok. So, I have just shown, some of the points. I have not shown all the points, but let us say these are the so my so my a b and c are basically this is a or a b and c ok. Now the 1 0 0 surface ok, so this intersects, intersects the a axis at 1 ok. Intersects it does not intersect the b or c axis ok.

So, if this is my a b and c, c directions these are the crystallographic directions a b and c. So, 100 will actually be parallel to the b and c axis and it will intersect the; a axis at 1. So, it will look something like this. So, it is parallel to the screen. So, it is parallel to the screen and it passes through, through this point it intersects the; a axis at 1; so this is the 100.

What about the 010? 010 will now, now this will be this will intersect the b axis at 1, but it will not intersect the a or c axis. So, the 010 will actually be ok, so it will intersect the; it will intersect the b axis, but at 1, but it will not intersect the a of the c, c axis ok.

So, so this is a 010 ok. Now because of the symmetry of the cubic system, because of the 3 fold symmetry of the cubic system, these two surfaces are equivalent or actually equivalent due to symmetry. So, 010 and 100 and let me add 001 are equivalent due to cubic symmetry ok.

So, these surfaces are equivalent due to cubic symmetry ok. And, so the notation used is. So, if I use the notation 100 ok, this corresponds to 100, 010 and 001. So, it corresponds to the set of all these all these 3 surfaces which are equivalent due to the cubic symmetry. So, in general the notation the notation h k l refers to set of equivalent lattice planes. And this is equivalent; this equivalence is due to the symmetry of the crystal ok. So, this equivalent is due to symmetry ok.

So, most simple example is the case of cubic where, where 100, 010, and 001 are equivalent ok. Alternatively I mean you could also have in cubic ok, you can also have let us say 110 is the same as 011, or it is the same as 101 ok. And again due to the cubic symmetry ok, these three are the same ok. There are many such examples you can take for a cubic system ok.

So, this represents a lattice a set of equivalent lattice planes sometimes this is called a family of, family of equivalent crystal planes ok. And correspondingly there is a notation for directions that is h k l with a square brackets; so this is the family of equivalent directions ok.

So, these are two additional rotations. We will not be using these too much, but it is what you might encounter these when you are reading literature or you are reading various books. So, that is why I wanted to mention these ok. So, with this, I will conclude the first lecture of week 8 ok.

Thank you.