Electron Diffraction and Imaging
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Lecture - 10
Tutorial - 01
Directional Planes and Zone Axes

Welcome you all to this course on Electron Diffraction and Imaging. In today's class we will discuss how to represent planes and directions in direct and reciprocal lattice, and the relationship between the directions and the planes in real and reciprocal lattice which are represented in zone block. In fact, about planes and directions especially with respect to direct lattice and reciprocal lattice, how they are represented theoretically. The theoretical aspects of it we have studied in a regular class. What I will do today is just I will tell you how to represent them, are how they are represented. For example, generally you know that we represent directions using a square bracket maybe u v w.

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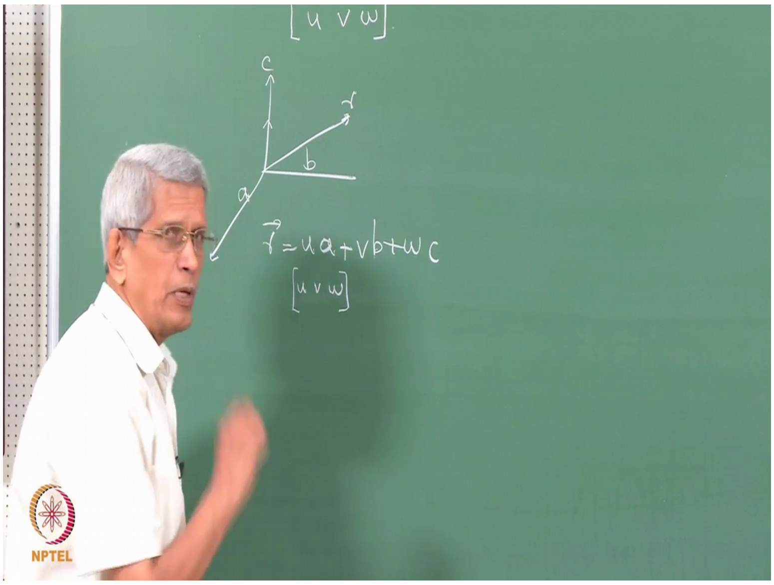

What it really means, in extra structure essentially is that from the coordinate system which we have chosen, for the crystal suppose this is a b and c direction. Any vector r if you wanted to find it is the vector.

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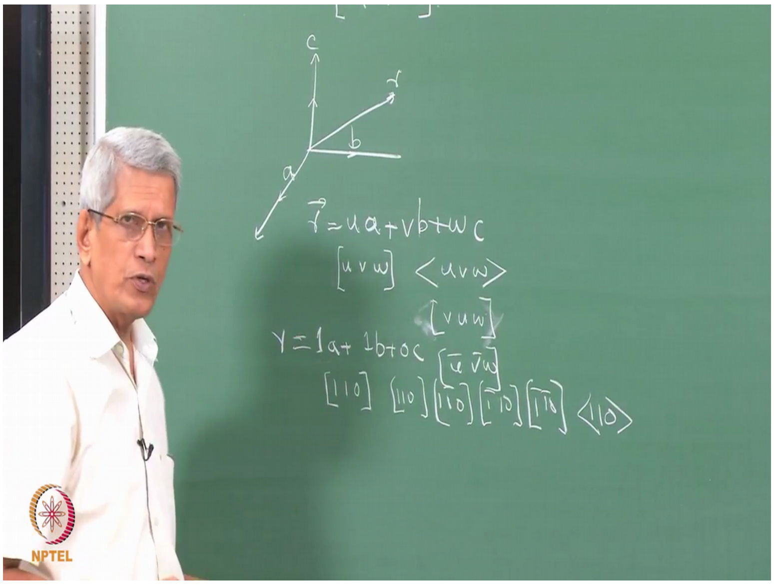

This is represented as a vector r equals u in to a plus v in to b plus w in to c. So, a b and c are nothing but vectors in the x y and the z direction in the crystal structure which we have chosen, and u v w are coefficients of this vector that is how much magnitude we have to move along a b and c. That is what it is represented this, we will be writing it just like this or u v w with a square bracket if you use a square bracket it means that it is a specific direction. And if you use a bracket with an arrow head u v w this means that it is the family of directions, which are include them. This could be this means that it could be essentially u v w, v u w all combinations or that if this could be a vector like this which includes all combinations plus it could be u bar v bar w.

All these direction look at these each one of them are distinct directions. This full family is represented with this simple. Let us take the case suppose it is only one unit vector in this direction x direction or a direction, and another in b direction and 0 in the z direction. Then the vector r will turn out to be 1 in to a plus 1 in to b plus 0 in to c. So, this vector itself as a representation, when we as we represent this as 1 1 0 this is how this direction is being represented if this includes all the directions 1 1 0 1 1 bar 0 and 1 bar 1 0 1 bar 1 bar 0, if you wanted to represent all of them together in single we be use this notation 1 1 0 this is how vectors sorry. So, essentially when we write 1 1 0 this representation is actually representing coefficients of the vector r. This one should always remember. How are the planes represented?

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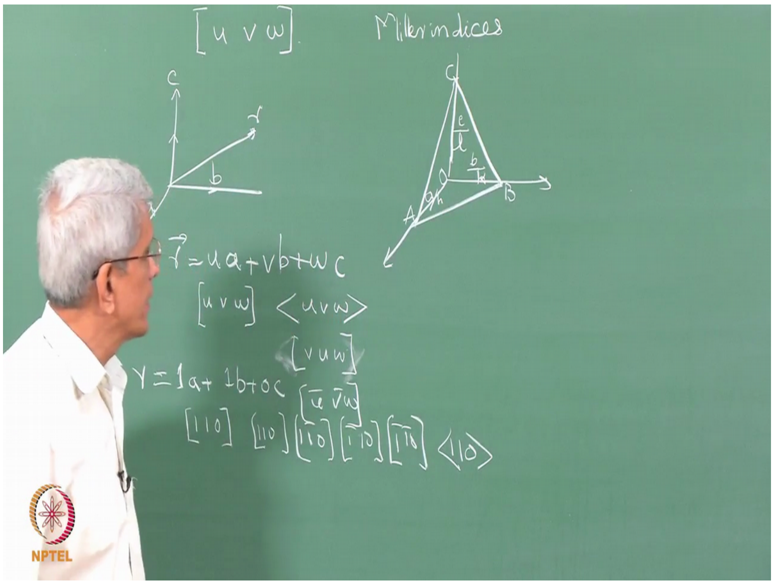

Planes are represented using what we called as miller indices. As you have studied to represent the plane, what we do it is, we choose that axis and draw the plane. Suppose this is a plane which is cutting along a axis an intercept which make a by h b by h is the intercept which b by k is the intercept which makes along the d axis and along this c direction, it makes an intercept c by n this is a b and c are the points at which the plane is cutting this axis.

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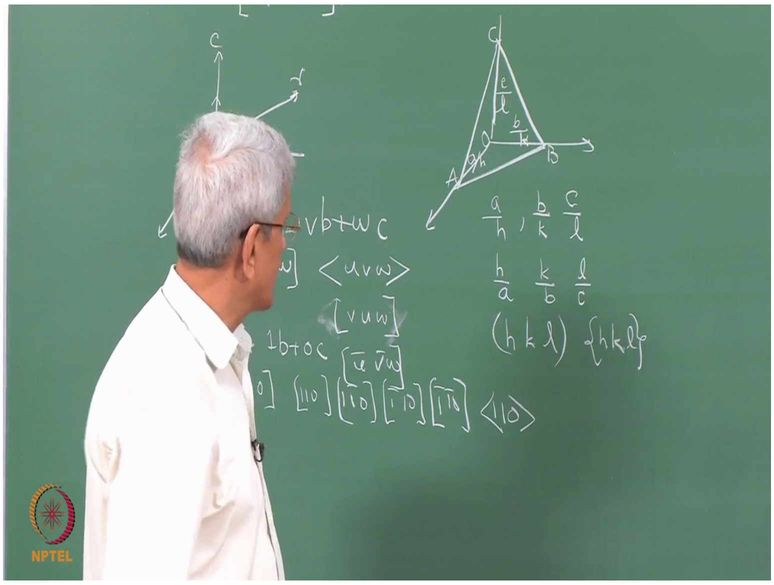

When the miller indices are we find out that intercepts which it is making it is a by h, then b by k and c by l. We find out the inverse of it then this will turn out to be h by a k by b l by c. Then removing the common factor then we will be writing h k l as the miller indices of this planes, and example if you wanted to represent a family of planes then we use curly brackets to represent h k l. This is how planes are represented, but what is essentially important and which one should always understand, key is that we write that, intercept which it makes as a by h b by k and c by l. At this point we have not talked about why we are doing.

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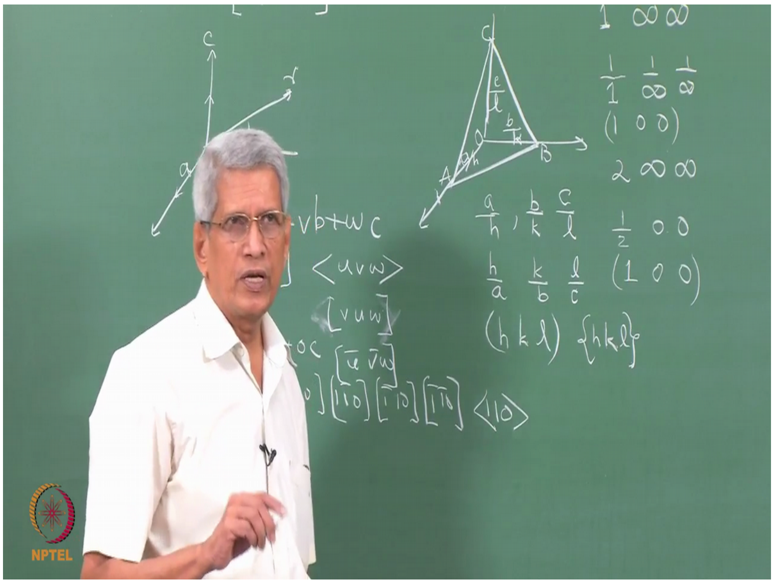

So, that is a special reason for this. This will become clear as we progress further. Let us take an example suppose along the x axis it makes an intercept of 1 unit. And along b and c axis it is not cutting it. So, the intercept which it makes it is only at infinity then we will be writing this as nothing but 1 by 1 1 by infinity the reciprocal of it 1 by infinity this will turn out to be 1 0 0. This is how this we represent as the miller indices of this plane. Just an another example suppose it is making an intersect not at 1 0 0 along the x axis, not at one unit instead make it at here suppose it is making and intercept somewhere here 2 units then this will become that intercept will become 2 infinity and infinity. Then it will be 1 by half 0 0 and miller indices are always represented not in fractions they are always represent in whole numbers; that means, that if we multiply it by 2, then this will turn out to be a fraction 1 0 0.

So, from this one aspect which becomes very clear is that irrespective of where it is cutting it along the x axis the miller indice of all these planes are 1 0 0. This is what you might have noticed that when planes which are parallel to each other, this plane is there suppose there is another plane which is where like this which cuts, this plane also will have the same miller indices. This property one can directly derive this way and this is one example to illustrate it. In this suppose we wanted to find out this vector a c, because in this plane a b c, we have vectors a c a b and b c.

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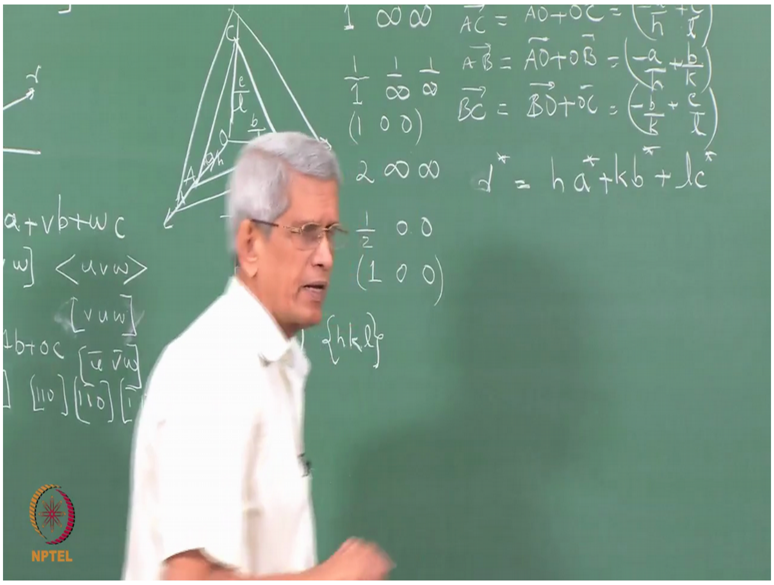

So, this can be represented A C will be represented as, A O plus O C. This will be nothing but will turn out to be minus a by h, plus c by l and A B is nothing but A O plus o b this will be again minus a by h plus b by k. And b c is nothing but B O plus O C this is B O is minus b by k plus c by l. If we consider a direction which is lying in this plane the direction normally a general direction be represented by the vector r equals u a plus v b plus w c. Since this vector is lying in the plane if we consider the plane normal, the plane normal is the angle between the plane normal and this direction has to be ninety degree. And in fact, these miller indices which we are using it is nothing but as you have studied in reciprocal space.

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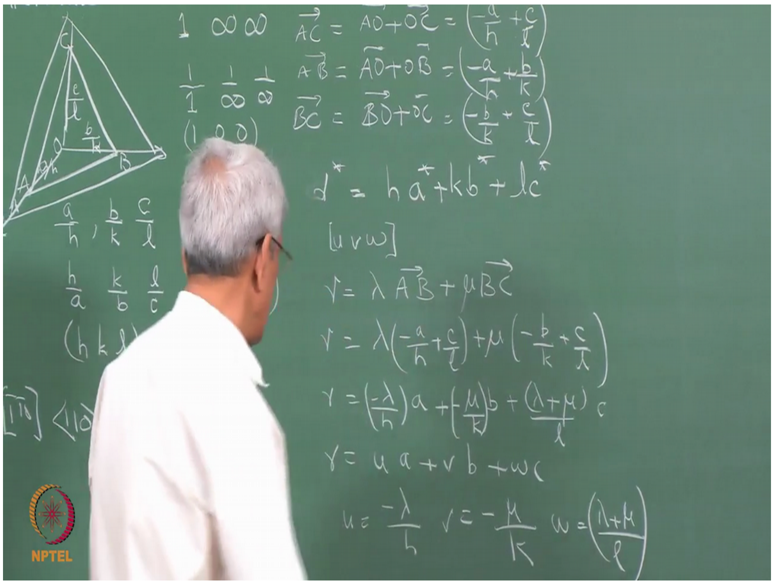

When we consider in a reciprocal space the vector is represented as r star, if we consider that will be h in to a star plus k in to b star plus l in to c star. The relationship between all these r and r star all these aspects you have studied in the class on reciprocal lattice.

What one should understand is that, if there is a vector which is lying in this particular plane. That vector as indices u v w. If you wanted to find out a vector which is the product of this vector that is u v w and h k l font though, how we can go about and do it is that, any vector which is lying in this plane r can be represented as some lambda in to a b, plus mu in to b c. In this way we can represent it correct lambda and mu are some constants which we have to find out. If we have a vector like this, then how do we represent r then, this a b vector we have defined it in this fashion. Then, the r will turn out to be lambda in to minus a by h plus c by l, plus mu in to b c will turn out to be minus b by k plus c by l.

From this if you try to find out r will be equal to lambda by h minus lambda by h, in to a minus plus minus mu b by k into b plus lambda plus mu by l into c. This is how it will turn out to be, but generally how do we define a vector r this we are presenting it as u in to a plus v in to b plus w in to c. So, now, we can find out that u equals minus lambda by h, v equals minus mu by k and w equals lambda plus mu by l.

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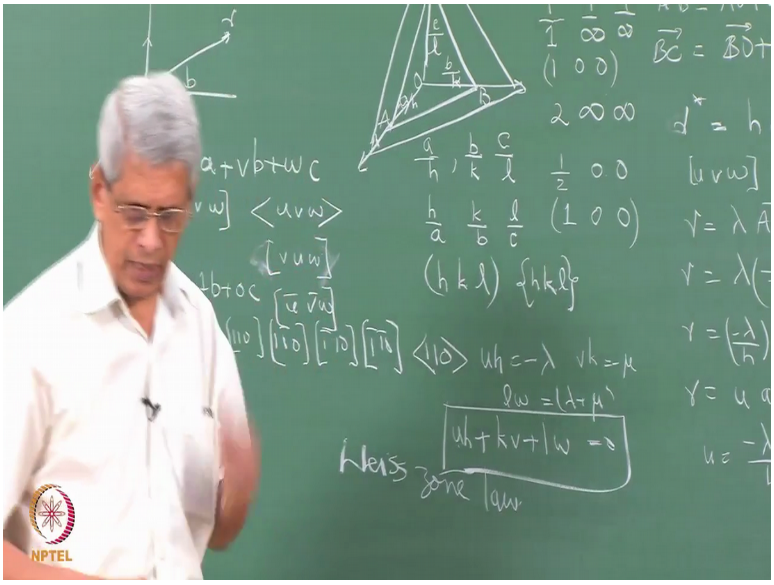

From this we can just write it that mu h equals minus lambda, v k equals minus mu. And l in to w equals lambda plus mu if we add both the right hand and the left hand side this will become u h plus k v plus l w equals 0. This simple derivation itself shows that the any direction which is lying in a particular plane, the dot product of it turns out to be 0. This is called as the Weiss this expression is called as the Weiss zone law.

Because one should understand what this zone law means. Here what we have considered is that we have considered one specific direction in a particular plane. There can be many directions which could be there.

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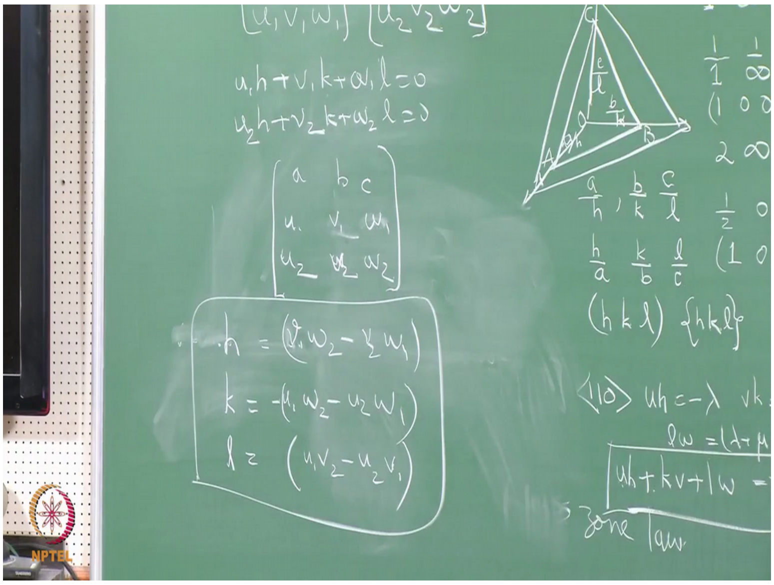

Suppose there is one direction u 1 v 1 w 1 with indices another direction with the u 2 v 2 w 2 both of this will satisfy that is own law, then we can write it as u 1 into h plus. If you add this together what we can find out is that if these 2 directions are known, then we can find out what this value of h k l. That can be done by just solving this equation or we can write it in another form, in which what we can do it is in tutorial it can be in a determinant form, then we can what we can do it is that, a b c u 1, u 2 u 1 v 1, w 1 u 2 v 2 w 2, then this vector r will be which we write it as, u then if you take this product the value because h k l, is the one which we represent the direction this will turn out to be, v 1 w 2 minus v 2 w 1 k will turn out to be, u 1 w 2 minus u 2 w 1, l will be u 1 v 2 minus u 2 v 1.

Using this formula also we can find out the miller that is if we know 2 directions 2 directions are given we wanted to find out what is the plane which is containing these 2 directions using this formula. You can find out the planes which contain these 2 directions miller indices of the planes could be determined using this formula. The converse essentially is that suppose we have 2 directions are there, 2 planes are given we wanted to find out that direction which contains that plane; that means, that the directions which are common to these planes. For example, suppose we have a one plane which is there like this.

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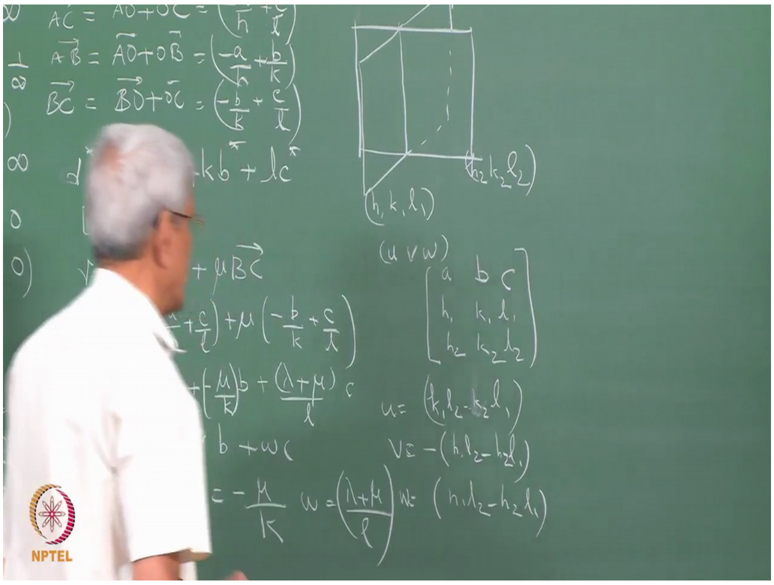

And there is another plane is cutting through this. This is the direction in which these 2 planes are intersecting; that means, that this direction is lying in the plane. Suppose this planes indices are h 1 k 1 l 1, and this particular plane is h 2 k 2 l 2, these 2 planes suppose it contains the indices of the one which we wanted to find out is u v w, then in that same way we can write a determinate. Here it will turn out to be, h 1 k 1 l 1, h 2 k 2 l 2. Then this will turn out to be u will turn out to be k 1 l 2, minus k 1 will minus k 2 l 1, we will turn out to be minus of h 1 l 2, minus h 2 l 1, w will turn out to be h 1 l 2, minus h 2 l 1.

This way we can represent the direction we can find out indices of direction which are contained on 2 planes, which are common to 2 planes. Another aspect which we have to consider is that, in all these derivations the way we have considered here if there is a way in which we are in a vectorial representation, we represent the direction and in the miller indices, form we represent the planes what is the other way in which these could be represented.

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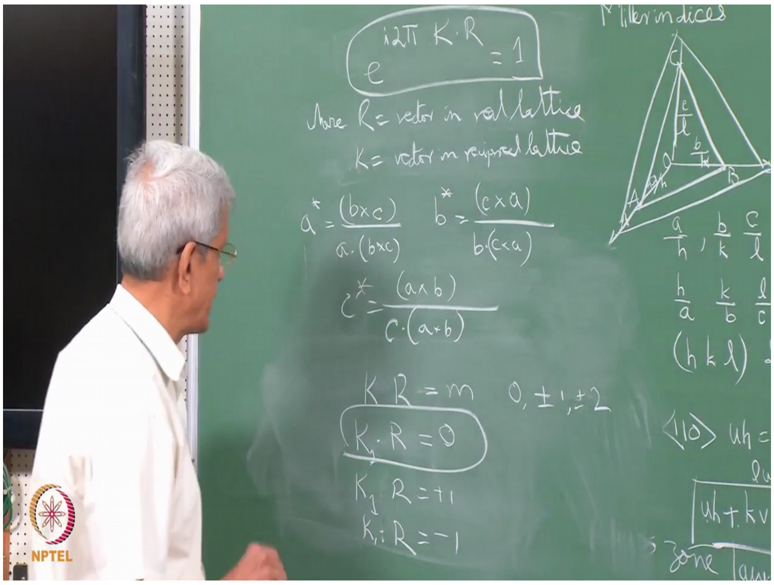

Because when we studied the diffraction the relations between the real and the reciprocal lattice, we derived see that one of the condition is that i 2 pi k dot r should be equal to 1, where r is a vector in real lattice k is a vector in reciprocal lattice. And then the derivations which we are derived are that relationship between real and reciprocal lattice is that if a star is a vector and the reciprocal lattice. This will be nothing but b cross c by a dot b cross c.

All these expressions have been derived. So, I am just writing the final answer divided by b dot c cross a, and c, c star equals a cross b then c dot a cross b. And the for this condition to be satisfied, k dot r has to be an integer m, where m can have value 0 r plus minus 1 plus minus 2 all values are possible. When we consider a case here when k is a specific vector, in reciprocal lattice, and then we are trying to find out the various values of r, for which this condition is being satisfied. This condition can be that suppose k 1 is a specific vector in reciprocal lattice. So, k 1 dot r can be 0, k 1 dot r can be equal to plus 1 k 1 dot r can be equal to minus 1.

All these things essentially mean that when k 1 dot r equals 0. This means that including for a point which is passing through the origin. This equation is satisfied; that means all the vectors which are perpendicular to the vector k 1, and passing through the origin. They satisfy this condition. When we say that they are perpendicular; that means, that all the plane which is represented by the vectors, these all the set of r vectors they define a particular plane. This is a plane which is passing through the origin.

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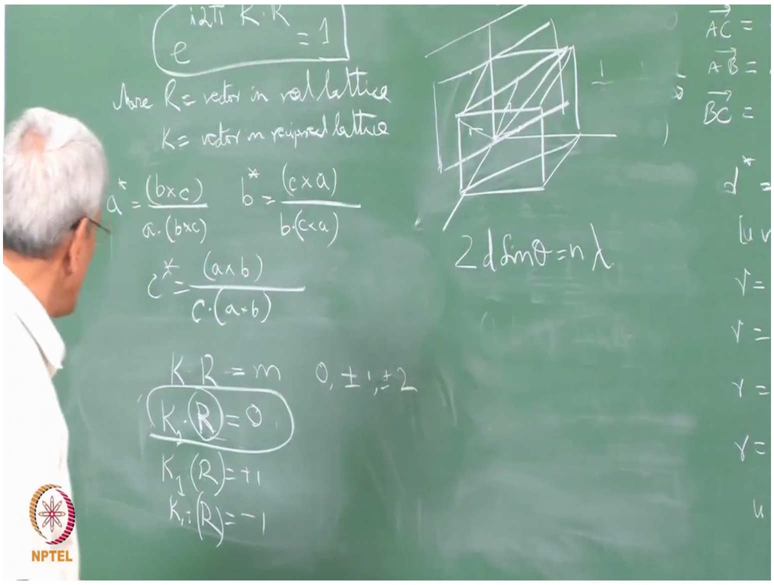

So, in crystallography terms if we try to represent this plane, is suppose we draw a unit cell of a lattice. Suppose we assume that there is a plane like this. The other one is a plane which is parallel to it and passing through this plane is also perpendicular to this specific plane which is passing through that origin. All the lattice points which are lying various lattice points which are lying on this plane, if you consider that as vectors then they will satisfy this condition. What does this k 1 dot r equal to plus 1 represent? It is essentially a plane like this where we have similar lattice points which are there from the origin; we can try to mark what is going to be the vectors which are corresponding to them.

All these vectors with respect to the k 1 vector which we have chosen, with respect to that and we know that this plane is perpendicular to the vector. So, this plane also which contains all these vectors they are all perpendicular to this vector k 1, so there such way. So, this is another set of r values this is another set of r values which will satisfy that is with respect to the planes which are behind this. Similarly, we can have series of planes which are in front as well as been. So, what finally, it represents is that each of this expression, tells that from these expression we can find a set of values of r which represents lattice points in those planes. And we know in diffraction these planes are the ones which are responsible for and diffraction to occur depending upon bodies the direction in which the beam is falling. And it should satisfy the condition 2 d sin theta should be equal to n lambda.

So, in real lattice it essentially means that, there are set of planes which are perpendicular to a vector k 1. This is essentially nothing but a reciprocal lattice vector. All the planes whether it passes through the origin or, it is parallel to each other for all of them. This reciprocal lattice vector remains the same this reciprocal lattice vector as you remember it is defined in terms of this r star is defined as h in to a star, plus k in to b star plus l in to c star.

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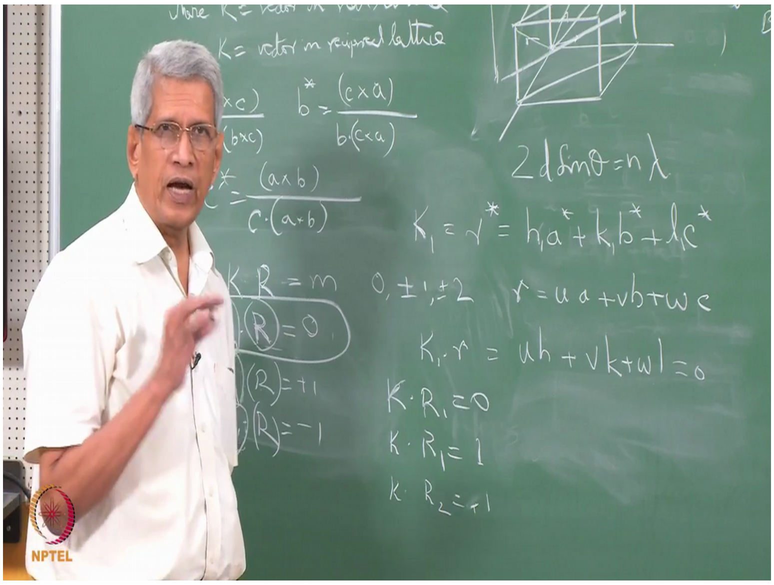

So, this k 1 is nothing but a there is a specific reciprocal lattice vector where the values can may be a specific value in this case it should be h 1 k 1 l 1. So, this is h k 1 l 1 which we used to define the miller indices of the planes are nothing but coefficients of the reciprocal lattice vector. This is what one should remember. Suppose we consider a vector r, which again i am coming at the same u a plus v b plus w c, this is how we define a vector in real space.

And a plane is represented as a plane normal and that can be nothing but in this particular form we can represent it. In this particular case if you try to find out the cross product the dot product of it because this one and this r is vector which is perpendicularly then needs to turn out to be u in to h plus v in to k plus w in to l and this should be equal to 0. So, this is what we call it as the Weiss zone law this way also we can derive the Weiss zone law. The other way if we look at it we set for this expression for a specific vector r, in the real lattice which we have chosen. We can have n number of reciprocal lattice points which also satisfy this condition k 1 dot r equals 0.

Then we will write is k dot r 1 equals 0, k dot r 1 equals 1, k dot r 2 equals plus 1. This is minus 1 like this we can have here these set of reciprocal lattice vectors they will be lying on a plane which is perpendicular to this direction r 1 in the real lattice. So, this represents nothing but a reciprocal lattice sheet. In the diffraction when you have studied you know that in the electron diffraction, it is a set of plane which is perpendicular to a particular direction which is responsible for diffraction. And we know that once the beam direction is defined we can identify for the electron diffraction using high energy electrons, what are the reciprocal lattice vectors which are lying in that specific plane will give rise to it. So, each of these this represents one plane, this represents an another plane which is nothing but the plane for which this k dot r 1 becomes plus 1, these represents an another plane where k dot r 2 becomes minus 1.

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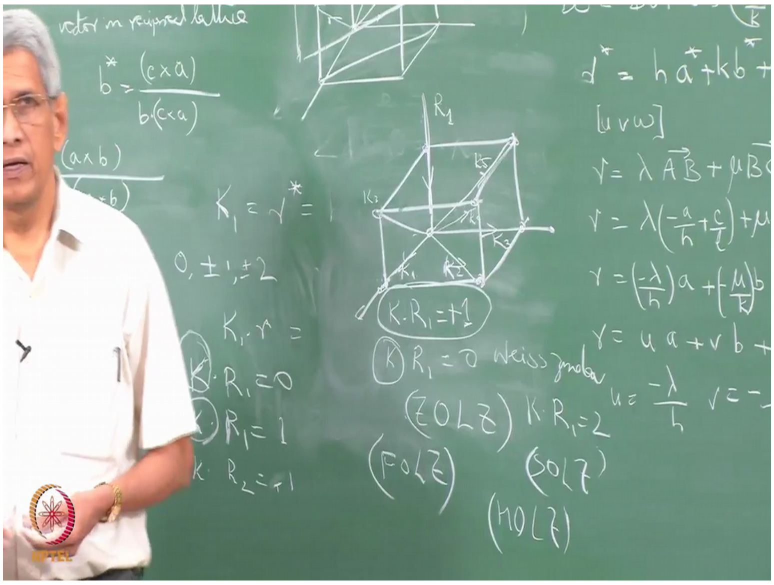

Essentially, what this represents is in terms of a reciprocal lattice if you draw a reciprocal lattice for a simple cubic cell. These are all the reciprocal lattice points if we consider it. And this is the direction for example, in which the beam is falling this represents r 1 the direction in the real lattice. Then with respect to a reciprocal lattice all these vectors this one this vector, this vector this if you have zone r 1 r 2, no this represents reciprocal lattice vectors k 1 k 2 k 3.

The dot product with respect to all these vectors turn out to be zero; that means, that all these vectors if you look at it these reciprocal lattice vectors are lying on a particular sheet. Similarly, if we consider this vector, this vector, this vector write it as k 3 k 4 k 5 all this set of reciprocal lattice vectors are lying on a plane which is parallel to it, but just above it and this set of one satisfy the condition k dot r 1 turns out to be 1. If you consider a prime which is below it, we can find out a set of reciprocal lattice points. Essentially the one which is there which satisfies this condition k dot r 1 equals 0. This we call it as the normally the Weiss zone law.

And this set of reciprocal lattice points this is called as the zeroth order Laue Weiss zone. This is how it is represented. So, all the reciprocal lattice vectors in this plane which is perpendicular to this beam direction, when they appear in the diffraction pattern we call it them as the zeroth order Laue Weiss zone all the reciprocal lattice vectors, which are there on this particular plane which satisfies this condition k 1 dot r 1 equal plus 1 they also satisfies this diffraction condition they are called as the first order Laue zone and the one which under the above that will be called as the second order that is k dot r 1 equals 2 this is called as the second order Laue zone in general these are called as the higher order Laue zones. These diffraction spots are generally seen in electron diffraction as well as an oscillating x ray diffraction we could see this sort of patterns could be seen here.

This condition when we consider it with respect to for a particular k 1 direction which is this is nothing but representing, the different types of planes that is the planes which are parallel to each other which are perpendicular to a particular direction k. That is the direction which is parallel to the plane normal. And they represent the different types of planes which are responsible for diffraction with respect to the diffraction pattern a specific direction, if we considered it, in the real lattice we can have different types of diffraction spots that condition is also represented by the same equation. In this particular case we are trying to find out the set of values of r for a specific value of k 1 which satisfies this equation; that means, that in this if we consider it almost all the planes which are responsible for diffraction, we could convert we could take it in to account suppose we consider another value of k.

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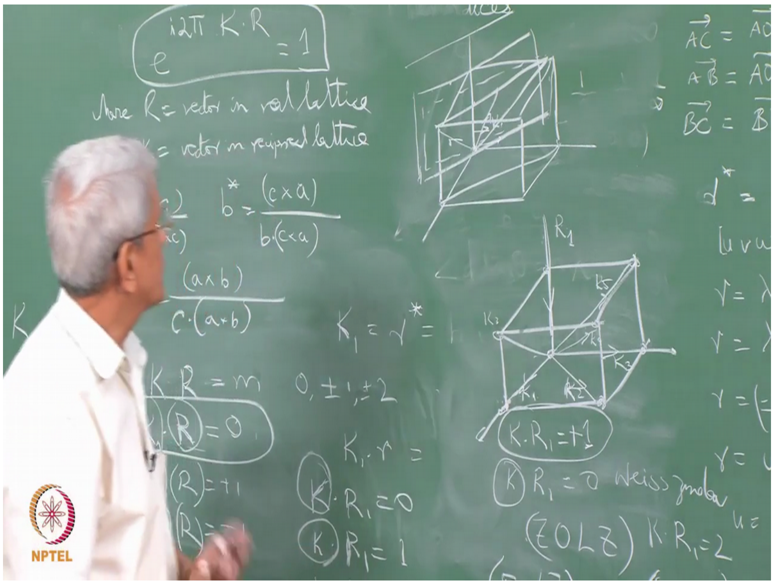

Instead of k 1 we take k 2, then what it will happen if and this will represent instead of this prime may be an another plane like this. Which is passing through the origin having a different k 1 vectors, they satisfy this condition; that means, all the planes which are parallel to this plane, on to which these various reciprocal lattice planes various real lattice points will be lying. So, essentially this condition represents the condition for the Bragg law what all the planes in real lattices are atom positions which are lying on different lattice planes which is going to participate in the diffraction. Here this represents given a specific direction in that beam.

What are the reciprocal lattice reflections which will be appearing in the diffraction, once the beam direction has been fixed that is what we are trying to find out? In this particular case once a particular reciprocal lattice vector has been chosen, what is what all the planes which are going to participate to give the diffraction spot. There is a subtle difference between these 2 statements that is what essentially this equation represents the condition for this one when k dot r equals to 0 that is what we call it as the Weiss zone law. This can be used both in real lattice as well as the reciprocal lattice. Then I had also shown how to find out the directions given a set of reciprocal lattice planes are it is equivalent to nothing but reciprocal like coefficients of reciprocal lattice vectors how to find out that direction, which is normal to the reciprocal lattice vectors.

Similarly, that same way given specific different directions, we can find out the direction of the reciprocal lattice vector or the miller indices of the plane which contain both the vectors. This is quite often used in diffraction to understand the diffraction and also in indexing this diffraction pattern.

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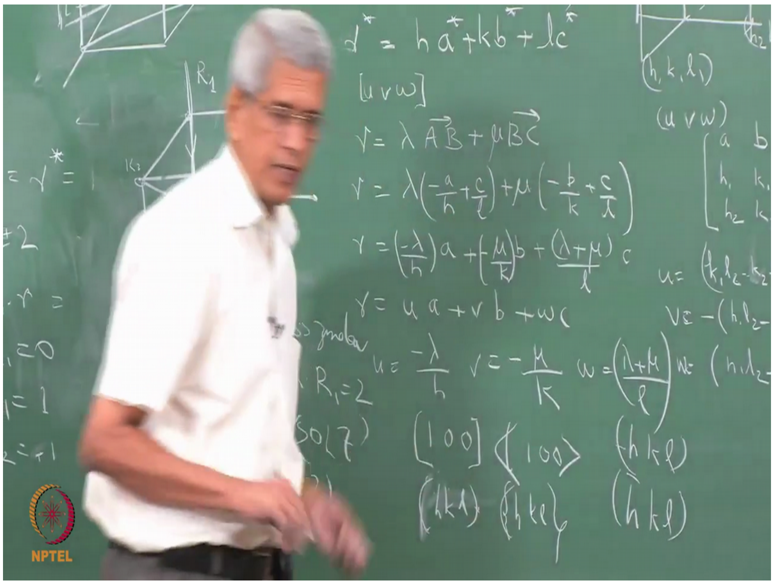

What is essentially important is that the apart from this expression as I mentioned in most of the time we use the terminology like square brackets to represent direction, then with arrows we represent family of direction, and this is u v w, this is h k l, we used to represent a plane with a normal bracket and with a curly bracket scale, these are indices which are used. And if you have to represent any direction minus h k l, how we do it is instead of writing minus h k l we write h bar k l this is the convention which is being followed to represent that plane.

These things one should remember, but all these indices you should remember that here this represents direction in real lattice. These represent coefficients of a direction which is represented in reciprocal lattice. I will stop here now.

Thank you.