X-Ray Crystallography
Prof. R. K. Ray
MN Dastur School of Materials Science and Engineering
Indian Institute of Engineering Science and Technology, Shibpur
Department of Metallurgical and Materials Engineering
Indian Institute of Technology, Madras

Lecture - 24
Tutorial 06
Discussion - Based on Forum Queries

Hello everyone. Welcome to this X-ray crystallographic course. In this tutorial what I will do is, I will try to address some of fewer queries what you have given through the feedback form. So, one of the first queries some student have asked how to do the miller indices or how to identify the miller indices for a non cubic crystal system. In fact, it is quite simple. You do not have to the procedures for identifying the miller indices are miller indices I mean directions, in the crystal system or miller indices that is a plane.

You do not require a separate for different crystal systems. The set of procedures given in the course is for any crystal of the form. So, what I will do is to since the student has asked that question, I will just write some of the procedures or some of the fundamentals I will just again once again I will write down in the blackboard. And then I will show that you can just easily mark the direction irrespective of the crystal systems and crystal planes and directions and so on.

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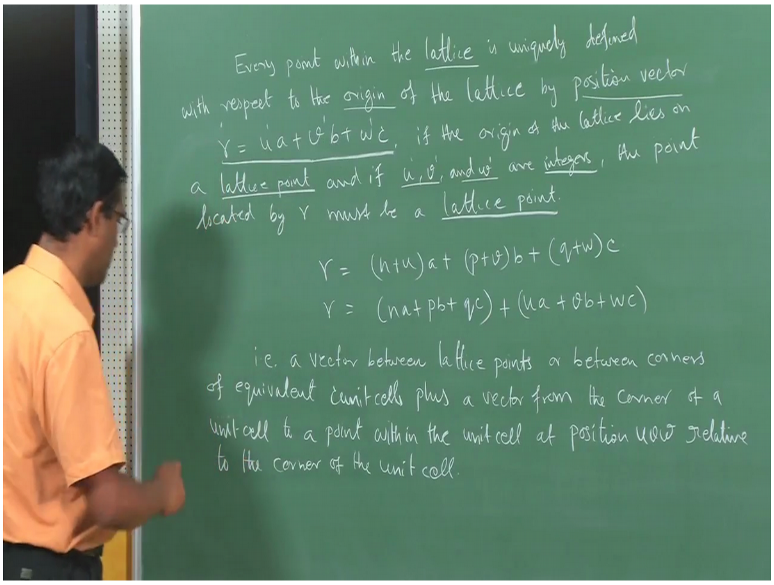

So, that is the first question I would like to address. So, first and foremost what you have to understand is, every point within the lattice is uniquely defined by with respect to the origin of the lattice by a position vector r is equal to u a u dash a plus v dash b plus w dash c. This is the position vector if the origin of the lattice lies on the lattice point and if u dash v dash and w dash are integers.

Then the point located by r must be a lattice point. So, this is the very fundamental definition of a position vector. So, if you understand this. So, you will be able to realise that you can simply identify the position vector in any lattice form in any of the lattices. So, you can also rewrite this equation in multiples of u v and w like this. So, what we have written is you can also write this equation with the multiples of integers the position vector can be written like this.

So, what I have written here is a vector between lattice points or between corners of equivalent unit cells plus a vector from the corner of the unit cell to a point within the unit cell at the position u v w relative to the corner of the unit cell. So, basically what you have to understand is you have to understand the position vector as well as lattice translation vector. You have to identify these 2 parameters then it is easy for you to look at the general lattice you can look at the general lattice of this kind. Let us consider.

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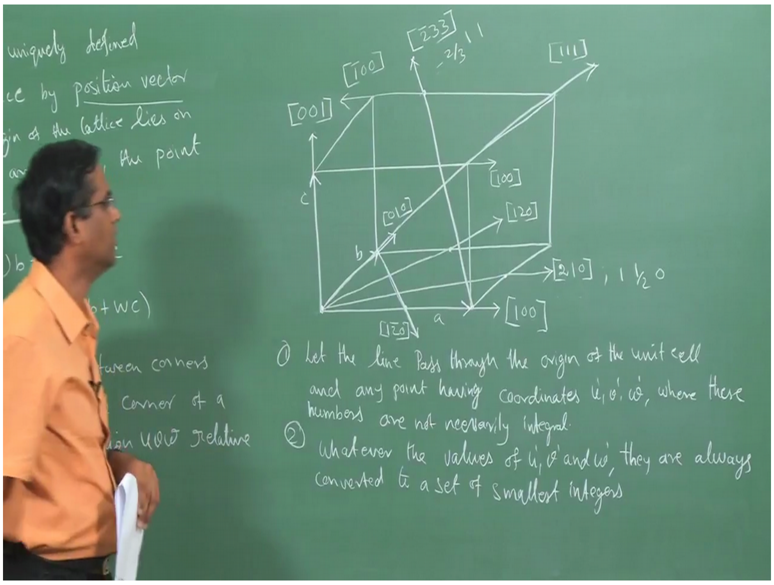

Let us consider this unit cell with the initially we will assume this is an origin and these are all the 3 perpendicular axis, that is a reference axis for identifying the direction of any kind.

What we will do is. So, direction to any unit cell or any crystal system you must have studied in this course that it is nothing but the coordinates you have to identify the coordinates with respect to which direction you were interested in. For example, if you take this direction: for example, if you look at these 2 simple directions. So, I do not have the coordinates of this is nothing but I have only in the z direction. I do not have coordinates from any other axis.

So, simply I can write like this. If you follow the steps what we have given in the course also you will find that you will come to this. What I will do is I will just simply draw some arbitrary directions in this unit cell, then we will check our procedures what we have learnt in the course.

So, the simplest directions, what you can identify in any arbitrary unit cell of this nature. You see that this 0 0 1 and 0 1 0 and this is 1 0 0 and this is again 1 0 0. These 2 are parallel indirections. So what you have to look at it let the line cross through the origin of the unit cell. And any point having the coordinate's u v w where these numbers are not necessarily integral. So, you do not have to worry about it not necessarily an integral. For example, if I draw a direction like this.

So, you look at these 2 directions we make sure that the direction is passing through the origin and then how do we get this suppose if you look at the coordinate of this, this is one half and then 0 because there is no z direction. So, one half 0 is been written as 1 2 0; that means, any fraction which comes we make it as a. So, that is what we do write we clear that fraction. So, let us write that point; so that you will not forget.

So, in this 2 cases you take the coordinates like here it is one, half and then 0 for this direction. So, you whatever the value you get for u v w. So, you convert them into smallest integers like this. So, that is how you do it. So, suppose if you change the direction suppose, if you have some negative direction. So, what you have to is either extend this unit cell to accommodate that negative direction for example, this positive side I can consider this as a negative side, I can extend this unit cell and then mark direction or mentally you can change the loc origin from within this unit cell to some other location depending upon the kind of direction you want to identify or determine.

For example if I will draw some negative direction in this unit cell itself, then you will appreciate that. So, I have a 2 situation here. So, this is about any fraction. So, you know that now. So, you can even write this coordinates, like 1 half 0 that you convert this convert this into this so that you will follow the similar procedure what about this direction. So, now, I have mentally changed the origin from this to here. So, this is my origin now. So, this direction we are interested. So, I am identifying this as 1 2 bar 0. How do we do that because you have the coordinates I have shifted the origin. So, it becomes a negative. And similarly you have origin shifted here for this direction. So, write the coordinates 2 by 3 1 1. Basically, the point is not in a not in half length by somewhere 2 by 3.

So, since the origin is here. So, I say that the coordinate is negative 2 by 3 1 1 for the other 2 units. So, you convert that into 2 bar 3 3. So, like that you can identify the coordinates even with the arbitrary point on any line. Only thing is you have to just remember that where you keep this origin, and then how your sign convention is you have to make the reference axis clear in your mind then you can always mark the direction without any problem, whether it is in plane or parallel to this axis or it could be like you know 1 1 1 like this. So, or it could be a fractional coordinates like this, or even the negative coordinates like this. Both of them you can identify and then the procedure is same, but only thing is you have to just remember that origin where you shit.

You can as I mentioned in the previous case like you can for realising the negative axis you can always extend this suppose you consider this as a positive axis you can extend this unit cell and then again draw this. Or mentally you change the origin and then with respect to origin you define a reference axis, where there is positive and negative and then follow the finding of the coordinates and then if it is a fraction you convert them in to a smallest integer and put them in a square bracket. So, that is a standard procedure. So, what I have not even defined what crystal system. This is this is just done this exercise is done on a arbitrary unit cell. So, similarly you can practice any systems till you become comfortable to identify, this the direction in a any arbitrary unit cells.

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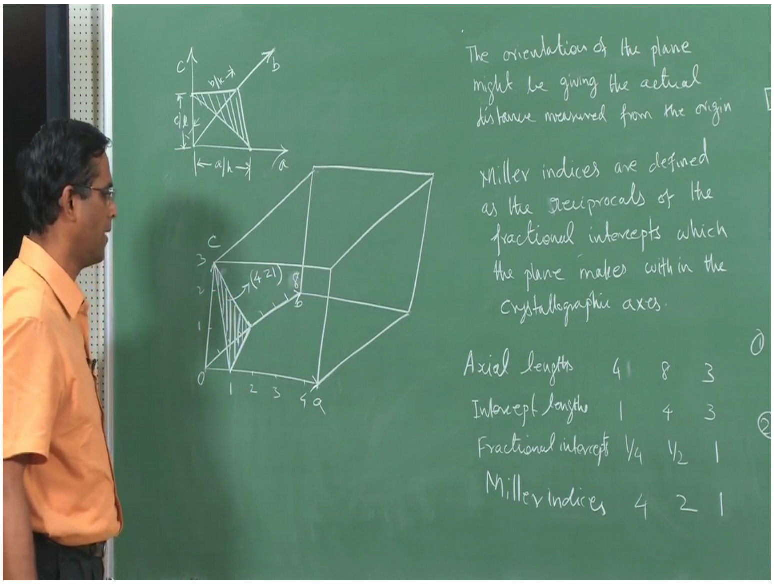

So, similarly we will look at the some of the example on the planes. So, what normally we do for identifying the miller indices of the plane, we always try to orient the plane or make the plane incline to the reference axis wherever the reference we have kept. Then we incline the plane into the 3 axis and then try to find out what are the intercept that plane is making on each reference axis; so finding out the intercepts. So, what we have I have taken again an a arbitrary unit cell where you have this axis reference axis a b and c. So, I have drawn a plane you can see that this plane is identified as a 4 2 1 plane.

If you go back and look at the procedures, what we have already done you can see that each axis has got a different divisions. So, basically we have just taken the intercept of we have arrived at this miller indices by calculating the intercepts, but before that what I would like to discuss with you is suppose. So, I am trying to explain, why we use certain procedure to I mean this particular procedure to arrive at the miller indices. Because as I just mentioned before, if you want look at the plane, if you want to identify with reference to this reference axis, a b c we always look at the intercepts and in fact, the orientation of the plane might be giving the actual distance measured from the origin we can always use that actual distance from the origin.

But the problem comes is when you have a plane which is parallel to the any one of axis then that plane will never make a an intercept with z axis. So, that is why the reciprocal of whatever the intercepts you get that comes because one by infinity is always make it as 0. And then you can put them into the curve bracket. So, that is the point you have understand otherwise whatever the actual distance measured from the origin. For example, here there could be a straight forward case, but then in order to avoid this parallel plane conflict because they will never make a particular intercept value with any of the axis.

So, that why the miller indices are defined as the reciprocals of the fractional. So, that is why the miller indices are defined as the reciprocals of the fractional intercepts which the plane makes within the crystallographic axis. Now, I have not again taken a any particular system of crystals, but it is shown in an arbitrary plane, but now you can see that as per the procedures laid down in the force, we will look at what are the axial lengths. So, you have if you look at this diagram the axial lengths are 4 8 and 3 in units any units, here I have not put any particular units. So, the intercept length is you can look at 1 4 and then 3; so fractions of this 1 by 4 1 by 2 and 1. So, if you make it smallest integers then this is 4 2 1. So, that we put in a bracket.

So, this is how the miller indices for a plane is identified. So, this is the same procedure what you have followed in the in the lecture that you have seen all that I have shown is some of the arbitrary crystal system, you can identify this and then you can practice and more different unit cells then this point will be much more clear.

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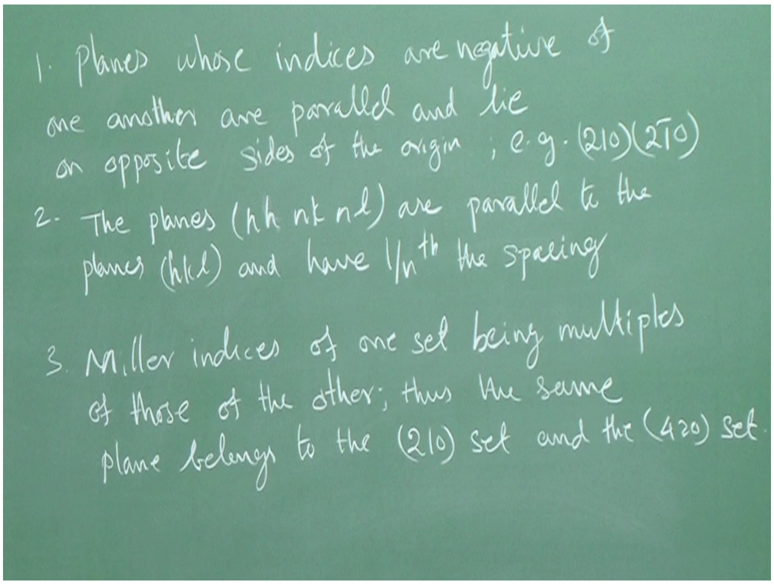

So, what I will do now. So, some of the points which you have to remember when we look at the miller indices of the crystal systems the planes, whose indices are negative of one another are parallel, and lie on opposite sides of the origin, for example, 2 and 0 2 and bar 1 0 there the same plane, but with opposite they are parallel planes, but with negative indices.

But planes n h n k n l are parallel to the planes h k l and have one by nth the spacing. So, that is you have some tough idea about how dense planes, they are miller indices of one set of one set being a multiples of those of the other has the same plane belongings to the, for example, 2 1 0s set and 4 2 0 set they are all parallel planes.

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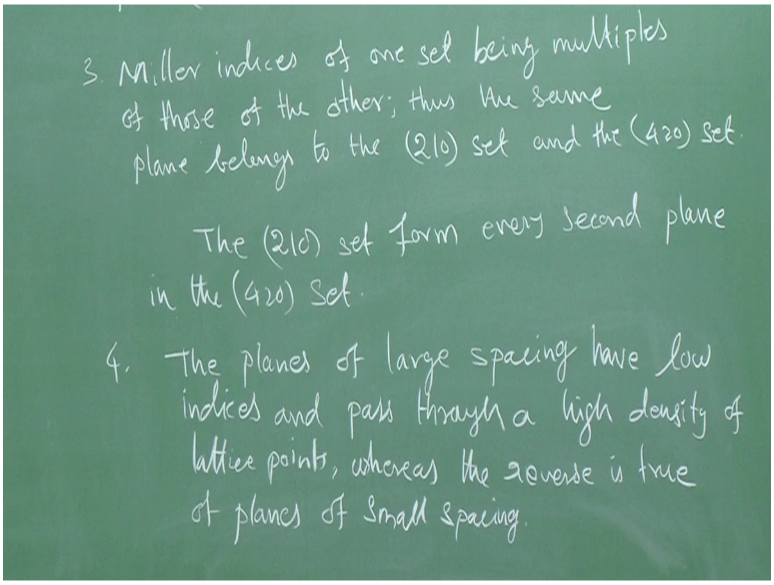

For example, these 2 will have the 2 1 0 for example, the 2 1 0 set every second plane in the 4 2 0 set. So, it will be a parallel planes. So, some of the things you have to remember, but another important thing is in a cubic system what you will have is the plane normals and all these perpendicular to the plane. That means, the direction and the plane or mutually perpendicular in the cubic system, but in other system it not necessarily true that is the only difference for example, in cubic system if you take 1 1 1 correction that will be perpendicular to 1 1 1 plane. Similarly for all the miller indices for in other crystal systems it is not necessarily true it will be something different.

So, that is the only thing you have to remember otherwise these points are still valid. So, another important point is to have about this miller indices is the planes of large spacing have low indices and pass through a high density of lattice points where as the reverse is true of planes of smaller spacings. So, you can have some idea about just looking at the miller indices. So, you can have some idea what I will is I will just draw the lattice; so that that is useful you can identify them by just looking at the lattice.

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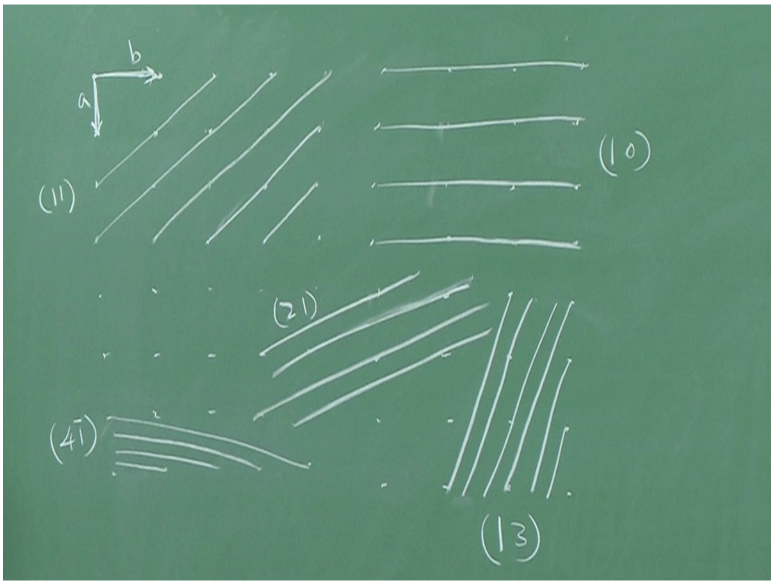

Suppose if I define this lattice, like b suppose if I have defined this lattice on the lattice translation vector like a and b. So, suppose if I want to identify these kind of plane this is 1 1 plane because we are talking about this is 1 1 plane because we are talking about 2 d. So, in 2 dimensions so this is 1 1; suppose if I extend this lattice further.

So, what I have done here is suppose if I looking at this spacing of this nature. So, it is like a 4 1 bar. Why 1 bar I have changed the direction and you see this is a 4 unit 1 2 3 4. So, it is 4 1 suppose if I extend this lattice further like this. So, this is 1 0 because it is only one direction. So, the other direction is 0 intercept I mean it is not connecting the other directions. So, it is 1 0 suppose if I extend this further I can show few more. So, what is have tried to show in this, lattice you see that the low indices plane have lattice spacing what I have just written here I have just shown in the schematic. So, the low index plane have higher spacing compared to the high index plane like this 4 1 1 0 and so on.

So, this will give you an idea by looking at the miller indices you can imagine high indices plane will be will be less have the less interplanar spacings. So, this I will conclude this session of the miller indices and directions. I hope you have some clarity on this to just do a practice on some of the exercises, I have demonstrated now I will move on to the next question the other students have asked to explain the brag law much more elaborately connecting the reciprocal lattice concepts.

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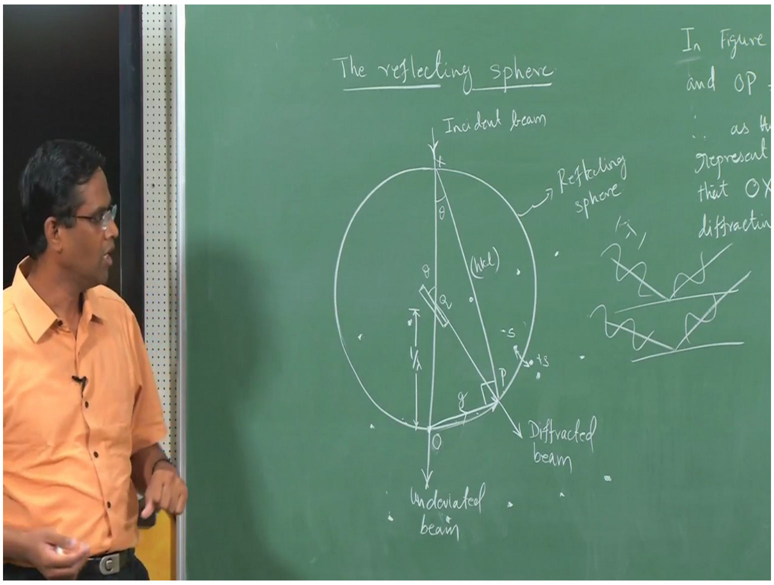

So, what I will lose I will redo that exercise on the board then we will discuss. So, now, let us look at the diagram you have already seen this twice. In fact, once I for the tutorial class and the other time you must have gone through the lectures. So, the question is con you explain the diffraction phenomena relating reciprocal lattice little more elaborately. So, that is concern from the some of the students.

So, what I have written here is the reflecting sphere is also called evolve sphere. So, it is a concept to it is an imaginary concept again like the stated in the lecture to connect the reciprocal lattice and the brag law there is a link between the reciprocal lattice and a brag law that is also you can use it as I mean via media to understand the diffraction phenomena. So, what happens is this is an you asking that this is an incident beam which is falling on a crystal and this is the diffracted beam and this is the undeviated beam or transmitted beam this phenomena is the same whether the incident beam is an electron or X-rays diffraction principles are the same. So, what you have to look at this is here what I have drawn is g is the reciprocal lattice vector that is what O P what I have written the reciprocal lattice vector g.

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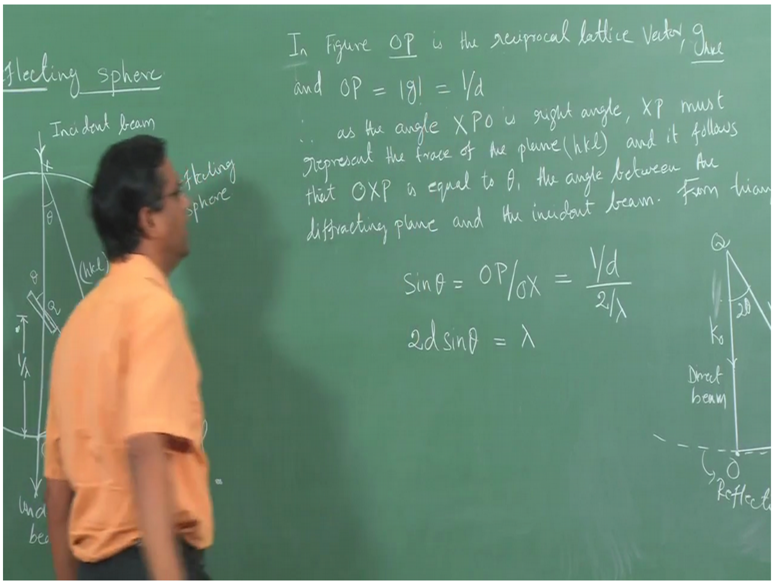

And you can the magnitude of g is 1 by d, d is the here interplanar distance. And if you look at the angle of X P o is right angle that is you have X P o is a right angle here, X P must be represent the trace of the plane that is X P the trace of the plane that is X P the trace of the plane is h k l and it follows that O X P is equal to theta where is the theta here O X P is theta here.

Again the theta is here the angle between the diffracting plane and the incident beam. So, from the triangle O X P O X P this is a triangle. So, you have sine theta is equal to O P by O X. How do we define OP here? O P is here it is g, g is nothing but one by d and O X is nothing but 2 by lambda this is one by lambda. So, this is 2 by lambda. So, we have written like this if you rearrange this then you get the standard brag law. So, if you look at this simple geometrical aspect, then it may look more mathematical rather than the concept, but then what you if you look at the schematic little more closely I have just drawn the spots to the background of this diagram. And this the circumference of this sphere is cut through only 2 points here, but this is a lattice an imaginary lattice which goes it is a infinite imaginary lattice.

But if you look at the sphere it cuts through only 2 points not the other points. So, another thing you have to understand, but now what we have done we have taken this reciprocal lattice vector. This vector which is nothing but one by d those things are there. So, now, you see that this is the direct beam and this is the diffracted beams. So, the distance between the direct beam and the diffracted beam we define as reciprocal lattice vector or diffraction vector we can also call it as a diffraction vector.

Now to understand this phenomena little more clear from this geometry, what we have done is the when the lambda is equal to 3D sine theta when the lambda is equal to 3D sine theta. Then this geometry is valid right or other way you can say that when this condition is satisfied when the lambda becomes 3D sine theta then the diffraction takes place because this sphere does not cut through any other point, but only this point; that means, whatever you see as a diffracted beam in a experiment has to obey this; that means, the wavelength of the incident radiation should be satisfying this condition.

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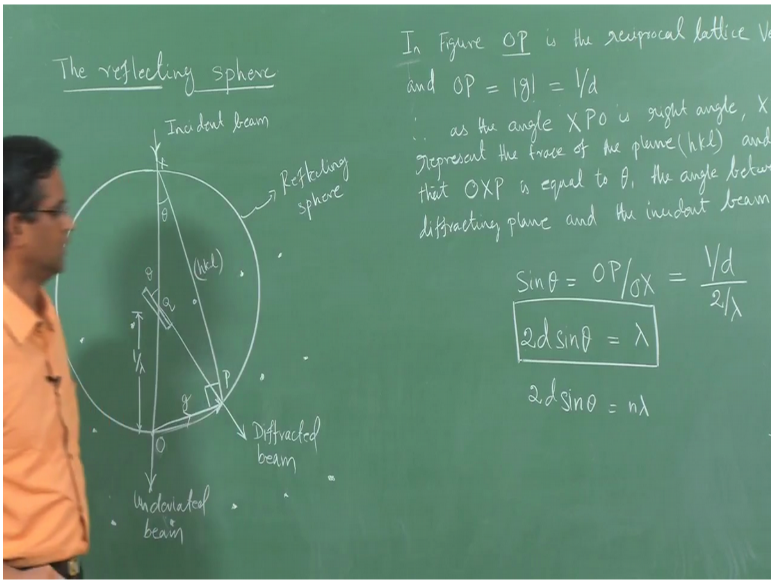

Then what happens when have or it could be like this n lambda. So, it could be an integral multiple of lambda, if it is of this nature then what happens the constructive interference takes place and which gives raise to the diffracted beam. So, if you look at the in the lecture notes much more closely what clearly shown in a parallel planes of like this incident beam and then this is diffracted beam like this.

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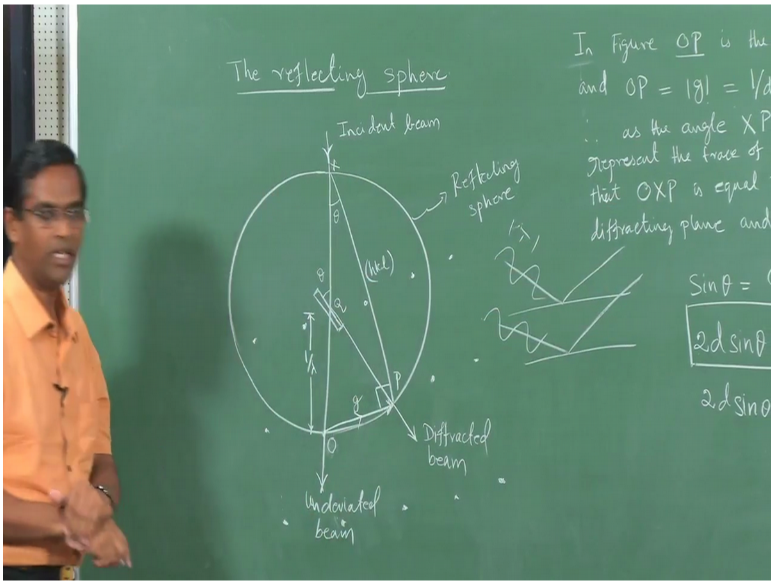

So, if you assume this like this is having some lambda particular lambda it will have some particular lambda, but when it is reflected that side when this condition satisfies then that incident is called diffraction that phenomena is called as diffraction.

That clearly demonstrated with this diagram unless the evolve sphere cuts through perfectly the reciprocal lattice vector, then you cannot call it as a exact diffraction then you may ask why we confuse this with this diagram, when we can understand this with the these kind of a parallel plane, and then it is at the diffracting beam and whether they are under same face then the constructive interference takes place and or not the idea is.

Suppose, if you have this evolve sphere as a reference when the evolve sphere exactly cuts this then it is exact diffraction or exact brag condition the theta is perfectly a brag angle it is on other ways you can always call that you can have a spot like this which is very close or somewhere in an imaginary not this particular lattice imagine, that you have a spot which is here or spot which is here some times it may come the reflection may come that will be called in exact brag condition. So, it this is the distance is measured as a deviation parameter called s.

So, this is positive s and one is negative s. So, deviation parameter that is not an exact brag condition, but it is a deviation from the brag condition. So in order to conceptually capture the idea of where is this exact brag condition is met and these evolve sphere construction really helps. So, wherever I have just drawn only a few reciprocal lattice points far off reference suppose you imagine that what ever the spot it cuts through or in this lattice. So, many suppose you assume that it cuts through so many points exactly on this. So, you will see highly densed diffracted spot in the diffractograms or in even if it is in electro electron diffraction you will see it in the screen lot more spots.

So, this is a sphere. So, it is a 3D projection here you assume that is a 3D if it cuts through the 3 dimensional lattice, so wherever the surface cuts through the exact lattice positions. So, so many spots will be appearing in diffract back focal plane or a diffracted plane. So, what you have to understand is suppose if this is away from this sphere where this way or that way your exact brag condition is not met. So, you will not have the a peak intensity of the diffracted beam. So, you will have very intensity of the diffracted beam. So, this can also be visualised in this form.

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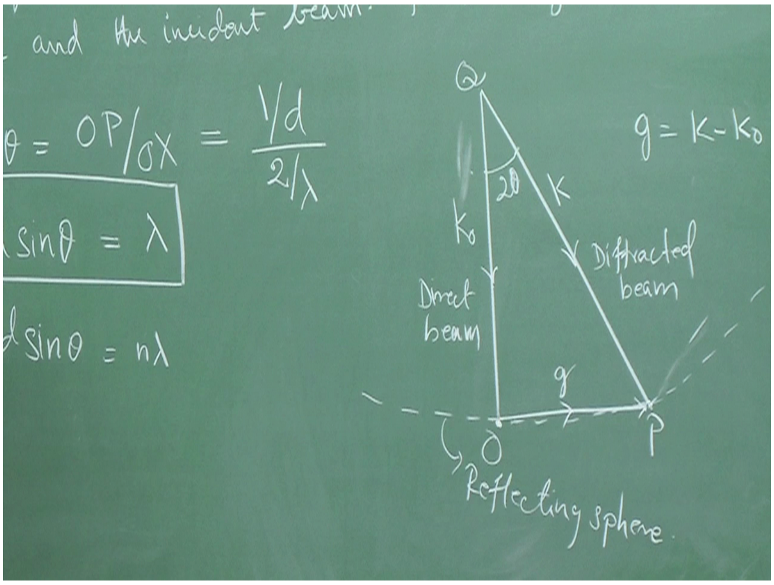

For example here it is a direct beam k not a diffracted beam is k. So, you have this diffraction vector g. So, vectorially we can show this as g is equal to k minus k not.

This is another way of showing a brag law in a vectorial form. So, so there are 2 things you have to keep in mind one is a geometry simple geometry the other is the physics behind this whole phenomena. So, both are you know imaginary concepts, but then helps to realise that what do you mean by exact brag condition, and how the you know the diffraction really connects the reciprocal lattice.

So, this is evolves sphere concept is a link between a brag law and a reciprocal lattice. So, that way it is most useful. So, another important point you can relate if you look at the X-ray diffractogram or XRD data you normally get very few number of peaks as compared to electron diffraction pattern in a semi crystal pattern, you will see lot more spots that is because the lambda is too small in an electron, I mean in an in a electron beam as compared to the X-ray wavelength.

So; that means, the evolve sphere is too big the lambda becomes smaller and smaller then your sphere becomes very big then it will cut through the surface of the evolve sphere will cut through n number of points. So, you see lot more diffraction spots in an electron diffraction as compared to X-ray diffraction, which gives very few diffracted spot or a peaks.

So, that is another way of visualising this diffraction phenomena using this evolves sphere, where it is very convincingly you can appreciate the useful of this diagram. So, look at this brag law by thinking about 2 aspects, one is geometry another is you can just look at by simple vector process or vector algebra, or you can just think of a some complete a physical phenomena we have to put all together, then your understanding of diffraction will be much better.