Introduction to Reciprocal Space
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Lecture -06
Diffraction Pattern
Worked Examples

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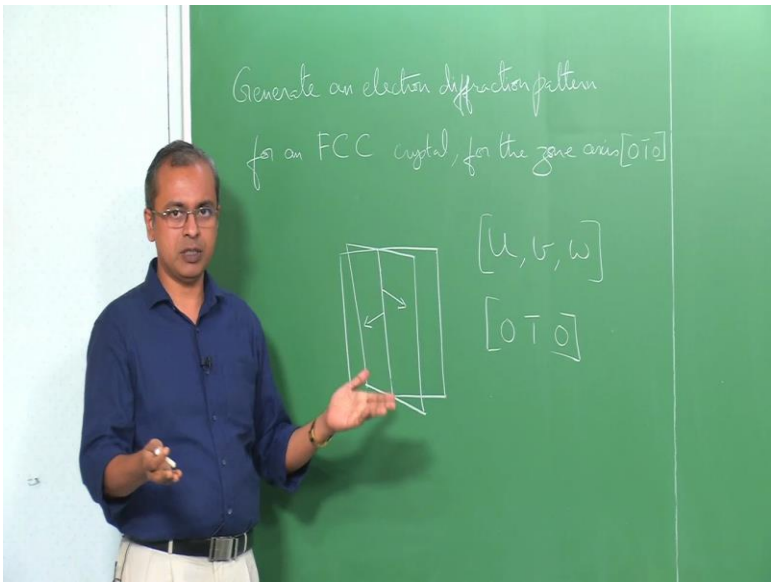

Hello today we are going to do a worked example, we have looked at diffraction, we have looked at reciprocal space. So, many of those concepts, we are now beginning to become familiar with. So, we are going to look at a worked example which relates you know some of the theory that we have discussed. With something that you may actually do experimentally which is to obtain diffraction patterns and then try to analyze those diffraction patterns.

So that is something that we as materials scientists, we do quite often in the lab. And one of the tools that we use quite regularly these days is the electron microscope. So, we are going to see how, what we have calculated, relates to a diffraction pattern that you would obtain off of a electron microscope. So, In fact we are going to actually generate a diffraction pattern and if you actually had a sample it would generate a pattern.

Similar to what we are going to put on the board okay. So that is the activity that we are going to do. So, I put down something like a question then we will look at various aspects of the question and in the end as we finish off, we will have a pattern which is the diffraction pattern that corresponds to that question. So, let us put down the question first okay. So, the question is this we want to generate an electron diffraction pattern.

An electron diffraction pattern in this case a spot pattern because we will assume it is a single crystal. We want to generate an electron diffraction pattern for an FCC crystal, for the zone axis 0 1 bar 0 okay. So, there are a lot of things that are specified here which maybe you may not have been familiar with or to some degree may have familiarity with. So, I will walk you through some of the terms.

And then we will actually do the pattern calculation and then yeah, so we will go about it. So, the first thing I want to point out is this term, so that there are a lot of things here, first is that, we are, I am talking of electron diffraction pattern, so there is some reason why I am indicating that. I am talking of a FCC which means face centered cubic crystal, so that also has some significance in the context of the question.

And the third thing that is of importance is this concept that it is along a particular zone axis. So, the issue is this when you take a single crystal and you obtain a diffraction pattern from it, that pattern is going to differ, based on how the crystal is oriented with respect to the radiation that is incident on it okay. So that is why this zone axis comes into being okay.

And the diffraction pattern that you get will also depend on the manner in which the diffraction pattern interacts with the crystal and that is why I have not spoken about electron diffraction. So that I will briefly indicate and the fact that it is an face centered cubic crystal also puts some additional specific specifications on it. So first let us start with something called the zone axis.

So, you may already be familiar with it, I will just very briefly show you what we are referring to when we say zone axis. So basically, we simply say that supposing you have a plane, I just draw a plane and let us say another plane intersects it. So naturally when two planes intersect if they are not parallel they are going to intersect at some point. And they will intersect along some line, so I will put that line down here and we will just say that this is another plane.

So, we now have two planes which are intersecting each other and they intersect along this line okay. So, now as you can imagine when you have a line that is on a plane, then the normal to that plane is going to be normal to that line. So, anything that is perpendicular to this plane will automatically be perpendicular to any line on that plane because that is how the plate is defined.

You have a plane does not matter which direction you draw lines on that plane. If you have a normal that normal will be normal to or any of those lines right. So, this line lies on this plane it also lies on the other plane. So, on both the planes this is a common line. So therefore, this line is perpendicular, so if I draw the perpendicular to this plane it is roughly in this direction okay. So that is perpendicular to this plane here, this normal that I have drawn here.

That is also going to be perpendicular to this common line. Similarly, if I take this plane here, the normal to it will be some in this direction and that naturally will also be perpendicular to this line because this line is common to this plane as well as this plane okay. So therefore, when you have two planes intersecting, the line of intersection is perpendicular to the normal two of each of those planes right.

So, this line, this common line is then referred to as the zone axis and you can actually have multiple planes, you can have a series of planes which go through this line. So, you can have several planes going through this line, common line or at least you can find such planes, which are all going through this common line. And for all of those planes this common line is referred to as the zone axis.

And in inverse way of saying it, all those planes are said to belong to this zone, there are planes of this zone okay. So, it is a direction, is a line in a crystal lattice, so you can specify it as you know saying u,v,w. You will say, you will specify a line in the crystal axis as u,v,w, so that is how it will end up coming, and it is a specific line. So, you have square brackets here, so therefore you will find that when you specify this.

You can say you can look at all the planes that are perpendicular to it and they will belong to this particular zone, so that is this u,v,w that we are referring to here in this particular question as 01 bar 0 okay. So, this is the zone axis that is there, now why we have picked the zone axis is

something we are going to look at in a moment. But at the moment this is, what we are referring to as zone axis.

I have just indicated to you, two planes and I have shown you the normal to it. Now we will okay, we will keep this picture in mind, we will come back to this in just a moment. What I am going to now draw is just a set of points which would then represent points in reciprocal space and I will also draw the Ewald's Sphere in this case it is two dimensional. So, an Ewald circle so to speak, which is the condition that we have identified as our diffraction condition.
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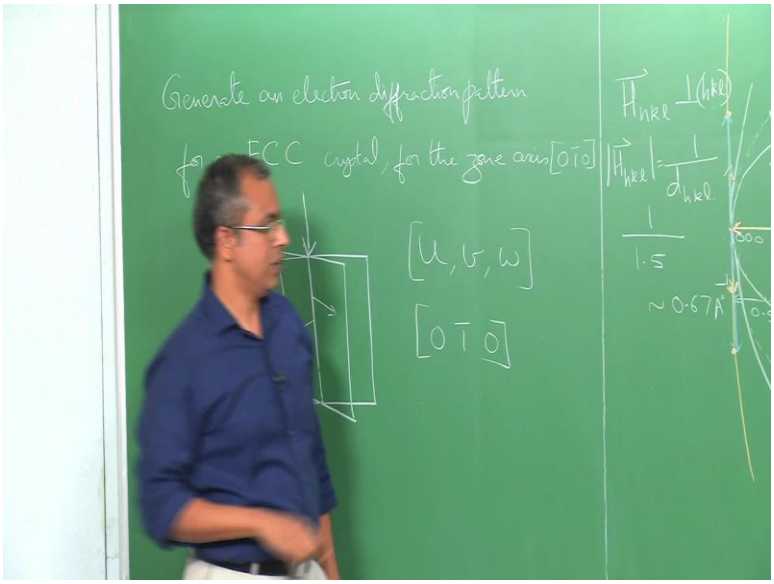

So, let us just draw some points here okay, so I have four by four grid okay, I will not just put one more point five, five by five grid, let us just do it. So, let us say these are points in reciprocal space, they are points corresponding to reciprocal lattice which corresponds to some real lattice. Let us not worry about which real lattice it is; it is these are valid reciprocal lattice points.

So, we discussed in our earlier classes that, so we would designate something as the origin which would then be 000. And if we have some radiation which is interacting with this lattice, we would draw the vector which would have 1 by lambda as its magnitude, 1 over lambda as the magnitude. And the direction, it would you just contact this 000 and then you would draw a circle with this as the center.

So, you would get a circle of this nature and wherever it happens to touch a reciprocal lattice point, so for example in this diagram the way I have drawn it seems to appears to touch this reciprocal lattice point. So, then the condition for diffraction is satisfied for this reciprocal lattice point, with respect to this radiation in this crystal. So that is how we have seen it, so this is a large, this is a circle that I have drawn.

Now the point to remember is, one additional detail we will add here, which is that as I mentioned once before in one of our earlier classes, you have a choice here, you have a crystal which belongs to the sample. So naturally you can keep changing from sample to sample and therefore you can have different crystals corresponding to them a different array of points would appear here.

You could also have independent of the sample, you can have different radiations incident on it. For each radiation, the wavelength would differ okay. So therefore, you can actually independently vary the radius of this circle or radius of the sphere in this case a circle, appearing as a circle on two dimensions. You can independently vary this sphere, and therefore for a given combination of crystal and wavelength of radiation incident on it.

Specific set of points would satisfy the Bragg condition, would satisfy the diffraction condition right. So that set of points is going to vary as you change the wavelength. It is not the same regardless of the wavelength. So, it is going to come based on the wavelength that you put on. So that is one point that we need to keep in mind.

But there is sort of an extreme end of this picture of, this basic concept that I have shown you, that you know, you can have a small circle, you can have a larger circle, when even larger circle and so on. Similar based on the wavelength and it is sort of an inverse picture because the larger the wave length this that you are putting incident on the sample the smaller is its reciprocal quantity.

So, this 1 by lambda becomes smaller and smaller as you as your actual lambda goes up. The opposite happens as you keep decreasing the wavelength, this radius keeps becoming larger and larger of the circle, so it becomes larger. And normally for example in x-ray diffraction, you will

have wavelengths of the order of say approximately in x, XRD, x-ray diffraction you will have wavelengths of the order of say 1.5 angstroms of that order.

So, copper k alpha is roughly in this dimension, this is a kind of quantity. The inter planar spacing is also of the order of 2 angstroms, approximately 2 angstroms. If you go to electron diffraction what happens is the wavelength that we use in electron diffraction, so this is lambda here, lambda is approximately 1.5 angstroms, lambda is off the order of something like 0.0 say 0.01 angstroms or 0.02 angstroms and so on okay.

So, you, what happens is, so you see these numbers here you have a 1.5 angstrom, you have a 2 angstrom and you have a 0.01 angstrom going to electron diffraction. I mentioned to you that these are what you are plotting in reciprocal space is an inverted quantity right. So, what, if it is large in real space it is small in reciprocal space. These two quantities are similar in real space, you have 1.5 angstroms, you have 2 angstroms.

They are similar order of magnitude, so you will see I know a set of points here and the spacing between these points which will be the inverse of this inter planar spacing, you are plotting the inverse of it. So, this is say if it is 2 angstroms the inter planar spacing, here is these inter planar spacing in real space. In this reciprocal space, it will be 0.5 angstrom inverse so that is what it is going to be right.

In reciprocal space 1 over 2, so that will be 0.5, so I will just say that this is 0.5 angstroms inverse. So that is so that is the dimension of this quantity in reciprocal space. The 1.5 angstroms would be inverse, so that is going to be in a similar order of magnitude here. So, if you do, so it will be roughly about you know .6, .7 angstrom inverse, so that is also of the same order of magnitude.

So, you will have a radius of that order, so 1 over 1.5, so roughly up approximately 0.67 angstrom inverse, so little larger than this .5 or something like that. So, you see when you use x-ray diffraction, the radius of the Ewald's Sphere that you generate is very similar in magnitude to the inter planar spacing that is present to the crystal okay. So that creates a certain type of, set of interactions that are possible and as you change the wavelength you start seeing different points.

In the different points satisfying the Bragg condition, however when you go to electron diffraction, you are using wavelengths that are 2 orders of magnitude that is different from the inter planar spacing right. So, if you have a wavelength of 0.01 angstroms the when you do the incident wave vector, this is the incident wave vector and which is, which has the magnitude 1 by lambda.

That 1 by lambda that incident wave vector, is now of the order of 100 angstrom inverse. The modulus of your incident wave vector is of the order of 100 angstrom inverse. So, it means if you have only .5 here, so you have to go 200 spacing's along this line, 200 spacing's along this line before you can, you know put the origin or the center of the sphere right.

So right now, for example I have no, I have put it at little over 1, 1 and a half for this particular, I know wavelength you would get for XRD you would see something like this. That is notionally okay, may not be an exact thing, so that is the center here. So that is the sphere with center here corresponding to the wavelength 2 angstrom, 1.5 angstroms wavelength okay. So that is for x-ray diffraction this would be the center and with respect to that, you would have this wavelength.

Some other wavelengths which would be slightly smaller would have a little larger wave vector and would generate that sphere that we originally drew. What I am telling you is that when you use electron diffraction, you are not going to go, at the center is not going to be just one or two reciprocal lattice vector spacing's. You have to go 200 times, 200 spacing's along this line before you reach the center okay.

So, you will have to go very far, very, very far on this board. So, you probably will have to exceed this board, well past this, the length of this board before you reach the center of the Ewald's sphere corresponding to the wavelength of 0.01 angstroms okay. So, but that does not change the condition for diffraction. The condition for diffraction is still the same. The condition of diffraction, for diffraction simply states that.

Whenever the Ewald's sphere touches a reciprocal lattice point, diffraction will occur right. So that condition of diffraction simply means that, you have to now generate the sphere corresponding to 100 angstrom inverse okay. 100 angstrom inverse and wherever that happens to touch a reciprocal lattice point you will see diffraction.

As you can see here, so given this condition, as you can see here when I go from a smaller radius to a larger radius, the curvature starts decreasing right, so that is inversely related, curvature is inversely related to radius. The smaller the radius the more curved it is, larger it becomes less and less curved. So, if you go to larger and larger and larger radius it almost starts becoming planar in the scale of this diagram right.

So, a larger radius would look something like that, so some larger radius, so these are the reciprocal lattice points. So those are reciprocal lattice points here. So, I have now drawn a part of a sphere which is larger in radius than even the one that I originally drew. So, if you continue this what normally happens is that when you go to electron diffraction kind of conditions?

Where you have 100 angstrom inverse as the no modulus of the wave vector that you are putting in the sphere corresponding to it, in this in the scale of this diagram, will almost look like a flat plane. It is a huge sphere of which you are seeing only a small section and in the scale of this diagram it looks like a flat line I mean it looks like a straight line or a plane in this if you look at it in three dimensions.

It is simply the surface, a small section of the surface of a very, very, very large sphere in the scale of this diagram okay. Because the radius of this sphere is know 200 times the spacing away and therefore in this scale of this image it looks like a flat and straight line. So that changes or that brings in certain very interesting situations into this analysis.

The main thing that it brings in is the fact that these are all now in this, these reciprocal lattice points that it intersects have a special property. You can see that corresponding to, so basically, I am only going to draw a part of this incident beam wave vector. So that is going to be something in, like this and it continues okay. So that is your incident beam vector, it just continues quite a bit like I said 200 spacing's that side.

So, I am going to draw part of it. Here this wave, this wave vector as you can see from the diagram that we have drawn, is perpendicular to this direction that you have here. It is basically perpendicular to this plane and off which we are only seeing a two-dimensional section, so you

are seeing a line. So therefore, all of these vectors that you see here, this is one vector, this would be another vector.

These are all vectors that are going from the origin 000 to specific reciprocal lattice points okay. So though all of those vectors are actually perpendicular to this vector that you see here and this vector this long vector is your incident beam vector okay. So, what do we observe, so the main points that we observe are when you use electron diffraction. The points that satisfy the diffraction condition appear to lie on a flat plane appear to lie on a flat plane.

The scale of this diagram and they are all points that are perpendicular to this incident beam direction okay. So, and what are these points they are reciprocal lattice vectors and what is the property of a reciprocal lattice vector. It is perpendicular to a plane in real space and the magnitude of it, is the inverse of the magnitude of the inter planar spacing right. So, we wrote Hhkl is perpendicular to hkl and modulus of Hhkl = 1 by dhkl.

These are the things that we wrote which is going to hold true does not matter what you are what your lattices etcetera. So, these are reciprocal lattice vectors, so therefore they are naturally perpendicular to those respective hkl planes and their magnitude is 1 by the spacing or 1 over the spacing of the that particular hkl plane. Now let us go back to our previous diagram you see here a perpendicular.

You see another perpendicular, so you automatically see that these are these can naturally represent directions in reciprocal space correct. Because they are perpendicular to respective planes, so this is perpendicular to this plane, this is perpendicular to this plane that I have drawn here. Therefore, they are valid reciprocal directions in the reciprocal space and if the magnitude is 1 over the spacing of the planes in this direction.

Then that would be a vector that would lead to a point in reciprocal lattice. But the interesting thing here is that they are all perpendicular to this line here that is the zone axis okay. So, we have reciprocal lattice vectors, directions of reciprocal lattice vectors are perpendicular to the zone axis. First, we independently drew this we had two planes intersecting; we said that the line that intersects that is common to them is the zone axis.

And we also notice that the perpendiculars to each of those planes are naturally also perpendicular to the zone axis. Now we also recognize the fact that these perpendiculars to those planes happen to be the directions in which the reciprocal lattice vectors would be, for those particular planes. Therefore, we recognize that the reciprocal lattice vectors would be perpendicular to the zone axis right.

Now let us go back to this figure here, we have a series of reciprocal lattice vectors and they are all perpendicular to this one line. Therefore, this one line coincides with the zone axis corresponding to these planes. In other words, if I want to take this picture and go back to that picture here, this is the beam direction right. This line that I am saying this line is commonly perpendicular to all of these points, all of these vectors.

This is the beam direction and these are reciprocal lattice vectors, so this image, if I move it to this picture here in real space, this is your beam direction, that is the direction of the beam and that coincides with the zone axis and then you have all the reciprocal lattice vectors, which are now perpendicular to it. They would down correspond to points which in the reciprocal space and that is how you would see.

So therefore, when you take electron diffraction the pattern of points that you see, represent points of a zone, they are all vectors which belong to that zone axis and the beam direction coincides with that zone axis. So that is the important point that we wish to note okay. So that is the peculiar thing about electron diffraction and how it shows you the points that you see there which are spot, spots those are all spots corresponding to the same zone right.

So now let us go back to this problem, we have here, so we understand the significance of electron diffraction in the context of this question. We also understand the significance of the zone axis which means the, this is the direction in which the beam is coming 01 bar 0. And corresponding to that we have an, we also have an FCC crystal for which in the 01 bar 0 direction the beam is incident and corresponding to that we want to generate the diffraction pattern.

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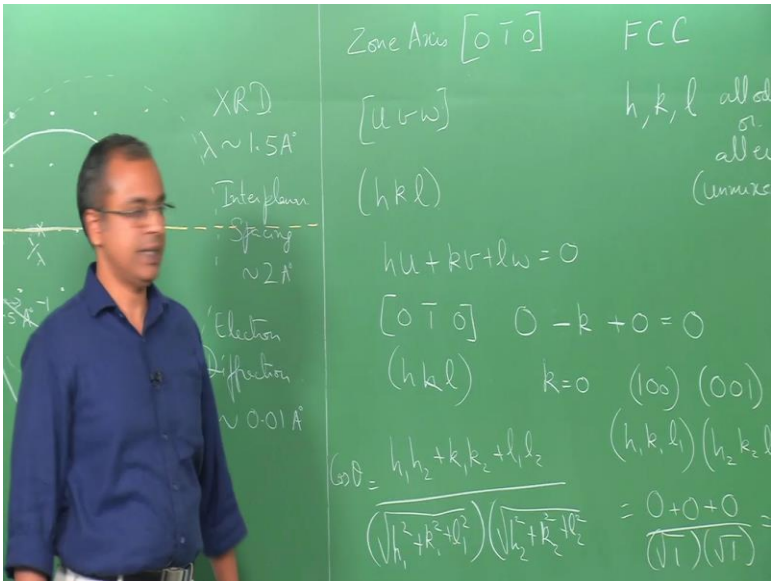

So, we will now do that there okay. So, we will now take the zone axis here again, zone axis is 01 bar 0, couple more concepts we will put in here which are very interesting. We also, I also mentioned here it is FCC okay. So, what I am actually going to do is actually, I am going to generate the reciprocal lattice points corresponding to this zone axis. Actually, for a simple cubic, initially I am going to do only for a simple cubic.

Then I am going to put a condition which says that certain of those points corresponding to simple cubic are not allowed for face centered cubic. So, you remove those points, what remains is the diffraction pattern of the face centered cubic. These are called extinction rules, there are something called extinction rules.

Simply because in a face centered structure you have additional atoms at some locations which would lead to additional cancellations or additional destructive interferences and therefore you will get a set of points if they were simple cubic. But some of those points get cancelled when you have face centered cubic. Another set of points get cancelled when you have body centered cubic or body centered structure face centered structure.

You have some cancellations going on additional cancellations. So, a simple cubic structure in this case will give you the super set of points that you can get and a subset of those points is what you will see in face centered cubic, another subset is what you will see in body centered cubic

okay. So, we will do it for simple cubic then we will eliminate or will highlight those points which are now valid for FCC.

Specifically, for FCC, the condition that is that holds for point for diffraction to be displayed by a plane or a set of planes is that the h, the k and the l values should either be all odd or all even should be all odd or all even. In this context then they also know instead of saying all odd or all even. They simply say unmixed meaning either all odd or all even. So, a 222 plane can give diffraction, a 242 can give you diffraction, 240 can give you diffraction.

But a 241 cannot give you diffraction, 101 cannot give you a diffraction things like that okay, so that is a problem, in the case of simple cubic such restriction is not there any value of hkl can potentially can give you a diffraction pattern okay, so potentially can give you over diffraction pattern.

So, when we do when we first draw the spot pattern will draw for simple cubic we will not worry about the individual values of hkl being unmixed odd or even. Then we will identify from that set only the ones that where hkl are either all odd or even and for that we will generate the, that will then that subset is then the diffraction pattern for the face centered cubic structure. So, this is the zone axis when something is a zone axis the planes that belong to the zone.

So, zone axis we will designate as uvw, the zone a, so that is the zone axis any plane hkl belongs to this zone, if hu+kv+lw = 0. So, this will not derive here we will simply accept this. There are derivations for this available, you can look there, look it up but this is straight forward relationship. So, if hu+kv+lw = 0 then that hkl plane belongs to this zone okay. And therefore, it has, you know it has a line this axis actually falls on that plane.

Like you saw for those two planes earlier, so now if you look at our zone axis that we are considering for this problem, we have 01 bar 0, so if I take any arbitrary hkl plane, what I am saying is h times 0 is 0, 0 - k + 0 should = 0. If I just do hu + kv + lw =0, so you have 0 -k +0 =0, so therefore for this to be equal to 0, we simply are requiring that k should be equal to 0 okay. So, all planes where k = 0, belong to the basically belong to the zone axis.

I have this, as you have this as the zone axis okay. So, I can write all these planes, so therefore quite simply you know if I have a 100 plane, it would belong to this zone axis or the zone would belong to this zone and I could also have 001 plane that would also belong to this zone right, so all of these would belong to this zone.

Now having come, so normally in reciprocal like in it since it is a vectorial you know it is a set of points that can be obtained by vectorial addition, it is sufficient if you obtain two points with something as the origin and then you can the two closest points to the origin and from there you can get all the other point simply by doing a vectorial addition, which is what we are going to do.

So, but to do that we need both the dimension we also need the angle between those two points. So, to get the angle when you have h1, so this is h1, k1, l1, so this is one plane that belongs to this zone for which that is the zone axis. And this is h2, k2, l2. So, the angle between those planes is simply h1h2 + k1k2+l1l2 divided by square root of h1 square + k1 square + l1 square multiplied with square root of h2 square + k2 square + l2 square.

So, this is what we will get and this is cos of the angle between, so this cos theta equals this right. So now I have those two quantities there, so if I just do this h1 square + k1 square + l1 square, square root of that is simply 1, so square root of 1 square +0 square + 0 square that is square root of 0 square + 0 square + 1 square both are square root 1.

So, I essentially have 0 +0 +0 square root of one into square root of 1 equals 0. Therefore, the angle between those two vectors is 90 degrees, so cos theta is 0, so therefore theta is 90 degrees.
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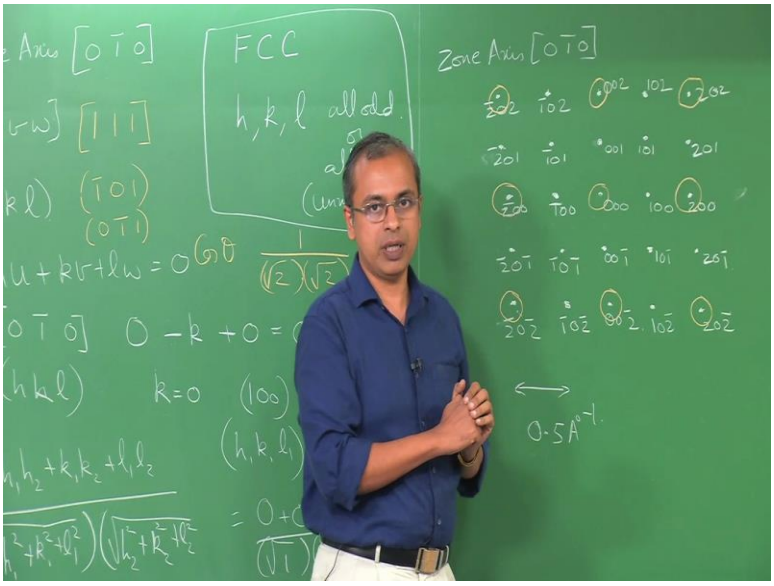

So therefore, I can set something as the origin and I will just draw, you know, so basically the first point that is, that I put down here, I can declare as let us say I declare this as 100, so I will call this 000, this is 100 and so this vector 000 to 100 the other vector has to be 90 degrees to this, so I just take a perpendicular point here. A direction perpendicular to it and I will call this yeah 10, 001 okay.

And now with this I will just draw a 5 by 5 grid and we just name all the points. So, I will just put here, point here, a point here and okay. If I great we will just stick to ye we will just stick to 5 by 5, so you have these two points here, so we just do that. So, square grid of 5 by 5 points okay. So, I have a 5 by 5 a square grid just drawn on the board we will just name the points. So, we have two points already identified here 100, 001.

So, we can just name the other point, so this would be a vectorial addition of these two, so this is 101 right and this is, I move two, two steps in this direction, so this is 200, this is bar 100, this is bar 200. Similarly, this is 002, this is 00 bar 1 in the negative direction, 00 bar 2 then we can name all the other points. So, this is 101 bar, this is 201 bar, so this is 102 bar and 202 bar. So, we can continue this, so this is 1 on the, so this is 2 on the x direction.

So, 201, 202 this is one along this direction but two along those that direction, so this is a 102 okay. So similarly, this would-be bar 101, this is bar 102, this is bar 201, bar 202 okay and we will finish these four points here. So, this is bar 10 bar 1, this is bar 20 bar 1, this is bar 20 bar 2

and bar 10 bar 2, yes, so that is what we have okay. So, the first number that you get will be the extent to which we are moving in this x direction.

So, -1 -, so this is all -1, this is all -2 and this is all 1, this is all 2 and the last number that you get is the extent to which we are moving up and down direction. So, all these numbers end with 1, all these numbers end with 2, all this number end with bar 1, all these numbers end with bar 2. So, this is how we have got the set of points. So, these are all the points please remember these are all the points without any further restriction.

All the points without any restrictions on h,k and l, I have not put except that they are all the points that correspond to that zone okay. So, they all belong to this zone, so zone axis for all these points is 0 bar 10. So that is the only restriction that is there all, so I have taken a cubic lattice and identified all the planes, that belong for whom this is the zone axis. And I have plotted them in reciprocal space.

And please remember that the only thing that I have not been, the directions are correct the only thing that I have not specifically put a value to is the length of that spacing. So just for our simplicity sake we will assume just, so that the numbers are convenient for us but it does not really. We will say that you know it was the inter planar spacing there was let us say it was 2 angstroms that is the example that we use there.

I think yeah 2 angstroms is what we used, so therefore all of this is .5 angstrom inverse, 0.5 angstrom inverse. So that is all it is, so we have got the dimension also, is now correct and the direction is correct because this is in at this supposed to be 90 degrees we found 2 directions. We found 100, 001 and we said that there, we found that the actual angle between them is 90 degrees and therefore we went ahead and built up this entire system.

So right so we have got all the points that belong to this zone and the dimensions are correct the directions are correct. So therefore, this is the set of points which are likely to be, which are the points basically that are on this line here, this is a line here in reality this should have been a plane and that is why the same plane I have now turned around and I am showing you that plane there.

So, this is the plane that is like this, this plane that is on this coming out of the face of the board going into the face of the board that same plane I put it flat on the board and that is what you see there that is the set of points is he there. So, corresponding to that diagram your beam direction is perpendicular to this board so the beam is falling on the sample like this and those are all the points that are possible right.

There you had the beam coming from, beam is coming from here and that is the plane, beam is coming from here that is the plane I just turned it around beam is coming from here this is the plane and that is what you see there, so that is the thing that you see. Now additionally I told you that our, so we have satisfied several things here. If you go back to our question here, we said electron diffraction, so wavelength is very small.

Therefore, the inverse of the wavelength the wave vector is very large. We found out the zone axis, we understood the meaning of the zone axis and therefore we were able to identify all those points that belong to that zone axis and we also found out that when diffraction occurs using electron diffraction. The points that you see are all the points that correspond to this zone axis.

So those points lie along this line, those are all perpendicular to the beam that is coming in. So that also we have done, so all these parameters we have taken into account. Only thing we have not yet accounted for is the fact that it is a face centered cubic lattice right. So, for that face centered cubic lattice, the additional condition that I told you is here.

In the case of a face centered cubic lattice, you for diffraction to occur in addition to the fact that those planes have to belong to the zone when you are using electron diffraction, in addition to that the condition. We want h, k and l to be either all or all even right. So now in our case, we are forced to look at only all even because we have got $k = 0$ that is the condition, that we got for the planes to be in that zone.

So, since k is forced to be 0 and so it is 0 in all the points that we have identified. We force to look at only the condition that all even, is what is going to get permitted for this particular combination of beam direction and sample, some other combination you could have got all odd also. So, in this particular case because the beam direction is like that you have $k=0$ and therefore we are only looking at all even points.

So, what are all those all even points we can just see here, so this is 1 odd 2 even, so it is not going to give you a diffraction spot, this is all even, so this will give you a diffraction spot, so I will just circle it, so that is going to give you a diffraction spot. Similarly, if you come here all even is here, this will give you a diffraction spot, this will give you a diffraction spot, diffraction spot, diffraction spot, this one here, this one here, and this one.

So, you now suddenly see that out of that you know full set of points that a cubic lattice would have given you. A specific subset is what the face centered cubic lattice will give you okay. So, this collection of points, this layout of points that you are seeing here, if you take that layout of points that would be the diffraction pattern that you will see when you do the diffraction of a face centered cubic crystal.

With the beam aligned such that it is lining up with the 01 bar 0 directions, so this is what you see as your diffraction pattern. And this is how it relates to what all the things that we have discussed in terms of reciprocal space and so on. So, the reciprocal lattice points that you generate are directly related to the diffraction pattern that you see and that is what we have shown I have shown you today.

And so, this is what happens the only additional detail that we have not put into this, is these scaling I have put the actual value here of 0.5 angstrom inverse. But as you can imagine any diagram you draw you can simply you know magnify this or it is a scale that you draw. So, I right now you know let us say this is 4 inches across. I have simply on this board, I have said four inches equal to 0.5 angstrom inverse.

You can simply say two inches equal to .5 angstrom inverse, in which case the whole thing would shrink a bit or you can expand it a bit. So that is like any other you know your magnifying order decreasing the magnification kind of thing. In the context of diffraction pattern, we talk of it as camera length. You can change the camera length and the changes, the extent to which this point spread out or come closer together.

But the layout of points, the angular layout of points would be exactly the same okay. And the pattern that you would see would look exactly the same right, so this is how it relates. So, this is a example that I wanted to work you through, so anytime you are given a particular lattice and

you are given the beam direction as something that coincides with the zone axis, a particular zone becomes the equivalent of a zone axis in that particular crystal.

It lines up with the zone axis in that crystal then corresponding to that you can generate the diffraction pattern. The steps that would be involved are of course first of all as just to summarize here, the steps that are involved is using the fact that the beam is coming along a particular zone axis. You identify, so that is uvw, if you, if any particular hkl has to belong to this, what would be the condition that would be required.

Mathematically it this is the condition that has to be satisfied, so given you have a particular value of zone axis, you have to figure out what are the restrictions on hkl for it to belong to that zone okay. So, for example I could pick another example where let us say I am looking at, give you another value here which would be let us say the 111 direction.

So, supposing you had a 111 direction then you would require, you know basically a particular value of h, k and l, such that the values work out to be 0. So, if you have, so for one 111 direction for example if you were looking at 111 direction, so the two planes that would then, two nearby planes that would satisfy this would-be a bar 101 and 0 bar 11, these two planes if you put in this zone axis you will get you to be able to satisfy a 0.

So, the first thing is you figure out at least two planes which belong to the zone axis, which are the nearest set of planes that you can think of. Smallest indices planes that you can think of that would satisfy this condition for that particular zone axis. Then you also, it is important to figure out what is the angle between those two planes. In our case it conveniently turned out to be 90 degrees.

So that is why you have a square layout of points there. In this particular case for example it will not turn out to be 90 degrees, so if you actually did this formula for it, so h1, h2 would be 0, k1, k2 would be 0 and l1, l2 would be 1, so you would have 1 and so this is cos theta and the square root of h square +k square + l square would be square root 2 square root of h square + k square + l square would be again square root 2.

So, this would-be root 2 times root 2, so this is 1 by 2, so theta is actually 60 degrees, cos 60 is half okay. So, if I add this as the zone axis the two planes that I would pick would be these two which would be very close from experience you can pick the lowest indices planes that would satisfy this condition of belonging to this zone and they would belong to the zone because they would satisfy this equation.

And then I also need to know the angle between them, so I should instead of drawing a square set of planes points that I have drawn here, I would said something as the origin, I would said something as the 1 bar 01 and then at 60 degrees to it, I would set the other one 01 bar 1. So those two I would set at 60 degrees. So, this would be twisted 60 degrees then I would generate all the points.

After having generated all the points I would then look at this additional condition the extinction condition which is whether they are all order all even and then generate all of these points. The subset, identify that subset which then satisfies the all the conditions required in the problem okay.

So, this is a nice worked example that I thought I should share with you. Which shows you how you go from a reciprocal lattice calculation to a diffraction pattern that you would actually see observe in the under an electron microscope. So, next time you see a diffraction pattern you need not be worried you can relate a lot of the things that we have discussed in our class and it will easily tell you how they relate to each other.

The in all this discussion there is one other point that I thought I would be interesting for you to keep in mind and that is simply that you know when you talk of real space and reciprocal space any quantity that is large in real space becomes very small in reciprocal space and vice versa. So that you have already seen I mean so a very small wavelength becomes a very large wave vector.

And correspondingly large relatively larger inter atomic spacing become a relatively smaller quantities in reciprocal space. So, what you see here is actually a slice in reciprocal space that you are off points. And these are points now because we are talking of a large single crystal where the dimensions are all large in all dimensions.

Supposing instead of a single crystal, large single crystal you had a thin film, so by definition a thin film is very small in one dimension, is very large in two dimensions right. So, corresponding to it, the intensity that you will see in, if you talk in terms of intensity of a spot in the in the reciprocal space. It actually becomes a rod, so where it is in large in two dimensions it becomes small in that dimension reciprocal space.

Another small thing in reciprocal space where it is thin it becomes a long rod okay. So that is something that you can at least keep in mind, you do not have to immediately I mean to do this you do not immediately need it. But just for you to you know really relate the thing that you see in the electron microscope to what you draw here.

When you see variations in intensity and so on those are some of the parameters that impact the variation in intensity and also you are taking a slice, so exactly where it slices through reciprocal space will give you that is why when you tilt the sample a little bit this way that way you will start seeing changes in intensity and so on.

And those are all the things that impact the intensity okay. So, we will not get into that detail too much but this is how what you have all the things that you have discussed relate to what you have, what you will actually see in an experiment. One other point that we should also note is that the origin, the choice of origin is arbitrary, so in fact the origin is also a point that would satisfy all of our conditions, which is that the h,k and l are all even.

For our particular problem because you have the 002 bar point here, this could have been chosen as origin. Then that would have been satisfied as the corresponding point. So, this then would be the final layout if you looked at the FCC with that being the zone axis. So, with this we will halt today and we will see in some other class. Thank you.