Introduction to Reciprocal Space
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Lecture -02
Condition for Diffraction

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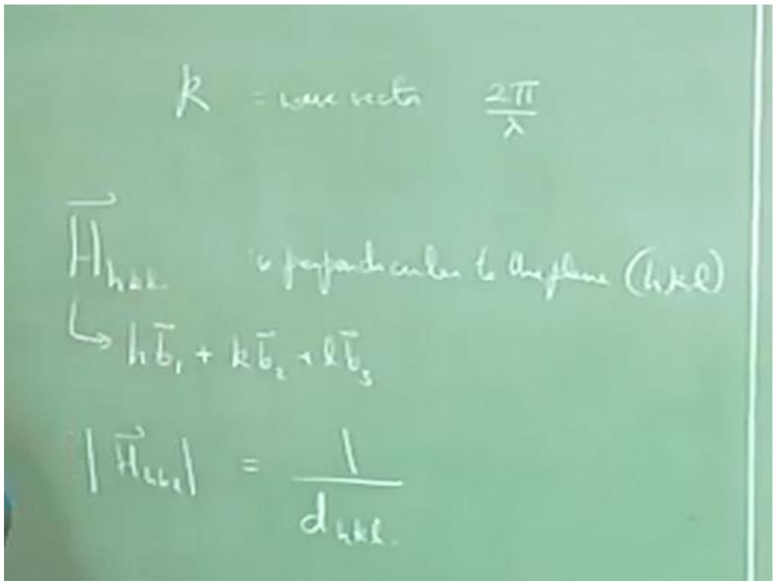

Since we want to get a feel for the different ways in which we can represent the interaction between waves and the crystalline structure and that in the solid and whichever works out most useful for us that is the description that we will use. We can actually we already have some description in the real space so to speak. In the conventional xyz space there is a description for how waves interact with the crystalline structure so we will begin there.

And we will look at that interaction because that is something that you are already familiar with from high school or even from early college classes. And then we will see how the same information can be represented in a reciprocal lattice formation okay. So, we will do that of course last class we looked at reciprocal lattice as an independent entity, we just basically said that we can, given a real lattice which has unit vectors a1, a2 and a3.

We can specifically create a reciprocal lattice which corresponds to this real lattice with the definition of the reciprocal lattice vectors, unit vectors in the reciprocal space b1, b2 and b3 having specific relationships to a1, a2 and a3 okay. So, we had a cross product b1 was a2 cross a3 by the volume of that unit cell and hence and similarly b2 and b3 were described.

On the basis of those definitions we found, we already found that for example in the reciprocal lattice, the vectors are designated by, we are standardly designating them using this Hhkl and the vector Hhkl, we found is perpendicular to the plane hkl okay. So, these are standard notations which you are familiar with the hkl plane based on the intercepts of the plane with the crystal lattice.

So hkl this is standard notation in material science it is standard notation and also in any other early physics that you have read this is standard notation. So, this is of course something in real space hkl plane the way we describe it and the way we you know visualize it and this is a vector in reciprocal space. And since the unit vectors in these two spaces have been, I mean defined or at least the reciprocal lattice vectors have been defined with respect to the real lattice vectors in a within a specific manner.

That is why we end up finding that this relationship holds true, that the reciprocal lattice vector hkl, which would then be hb1 + kb2 + lb3 okay. So this is what the hkl is okay, so and this where, this vector is going to be perpendicular to the hkl plane in real space so okay. So that is how it is and the modulus of Hhkl okay is simply 1 by dhkl, the spacing between these planes that is the value of this modulus of this okay.

So therefore, we find that both these relationships are I mean clearly indicate that there is some geometrical relationship between these two spaces that we have created. And that is being borne out by this these two relationships okay. So, these were the two major relationships that we derived last class after having defined our reciprocal lattice.

So today we are going to look at the interaction of the waves with a crystalline structure, periodic structure and we will first do that in the real space because that is something you are familiar with and then we will do that in this reciprocal space. And we will see that essentially the results are comparable and that we can draw some conclusions from that okay.
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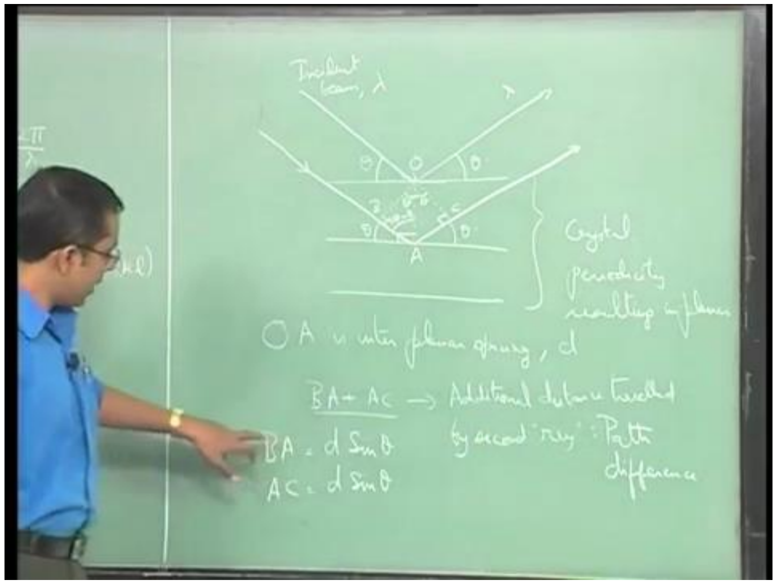

So, in real space we are conventionally basically say that you know we have a series of planes of atoms. As you are aware you know when we say planes of atoms that is just something for our convenience that we say. In principle atoms are occupying only periodic locations within the crystalline structure that is all they are. So, it is just a location it is an address for that atom so to speak and it stays there, within the context of our discussion.

The plane has such that we define is our convenience we just say that we along a certain plane we are seeing several atoms. So, we define that as a plane in the crystal structure. So that is how it is, so when we pick a plane when we draw it like this it is our definition that is that this is a plane right. So, we will take an incident beam of, so this is a periodic structure, so this is the crystal structure. The crystal periodicity permits us to define this plane, so we have an incident beam of wavelength lambda.

So, it is coming in with some wavelength lambda. Then we look at a diffracted beam also at wavelengths lambda. So, we are assuming that the interaction is such that the wavelength is not being modified in any way. The incident beam is incident at some angle theta okay, and we will say this is also theta, we will look to see at that the diffracted beam in that direction and see what is happening. So, we will see for interference purposes.

When we say diffraction, we are looking to see if there is constructive interference from a collection of waves okay. So, it is not just the single way, we are interested, we will see also what happens with, when you are sending a beam of waves. We have said that this is a beam, so there is an adjacent wave also coming in which will perhaps interact with this second layer and come out. So, we will look at a similar wave which comes down here.

So, this is again an incident wave and this is a diffracted wave and again these angles are still theta. Now this spacing here between this point and this point, we will just say this is O this is A. So, OA is inter planar spacing which we standardly designate as d, d is the inter planar spacing okay. So, this is what the OA is, this distance between it is a planar spacing between these planes.

So, if you see we would like to first find out what is the path difference between this wave and this wave. Since they are all coming in such that they are in phase both the waves are in phase. So, we will look at the path difference here. So, this is the additional distance being travelled by the wave that is coming to the second plane and this is the additional distance. So, this plus this, so we will just say that we call this B and this is C.

So, BA + AC is the additional distance being travelled by the wave that is coming to the second plane, relative to the first plane okay. So, this, up to here they are exactly in phase, second wave travels this additional distance, travels this additional distance then from here on they are all travelling the same distance these two waves are travelling same. So, this is the additional distance being travelled.

So if you see here since this is theta and this is 90 degrees, this line has got to be perpendicular to them, only then this is the spacing, so this is 90 degrees right and this is 90 - theta. So, this is theta, so therefore this alone is 90 - theta right, therefore this is theta. Similarly, this is also theta right, so this angle is theta therefore this angle in this triangle this angle and this whole angle is 90 degrees therefore the remaining angle here is 90 – theta.

Therefore, the third angle here and again this is 90 degrees, therefore that is theta. So, if you say this is d, this is d which is OA is the planar spacing d. Then OB or I am sorry the AB is simply d sine theta, that is a straight forward the trigonometric relationship. So, BA = d sine theta, that is theta and so this is d, d sine theta would give us this distance. And similarly, d sine theta would also give us this distance because it is the same relationship here.

This is d and sine theta of that would be would bring it here d sine theta would bring it here. So similarly, AC is also d sine theta right. So therefore, so this is the additional second ray if you want to call it that, second ray of the beam of rays. So, the total additional distance, our path difference, this is also called path difference okay. So, path difference is BA + AC each is d sine theta. So therefore, the total path difference is simply 2d sine theta.

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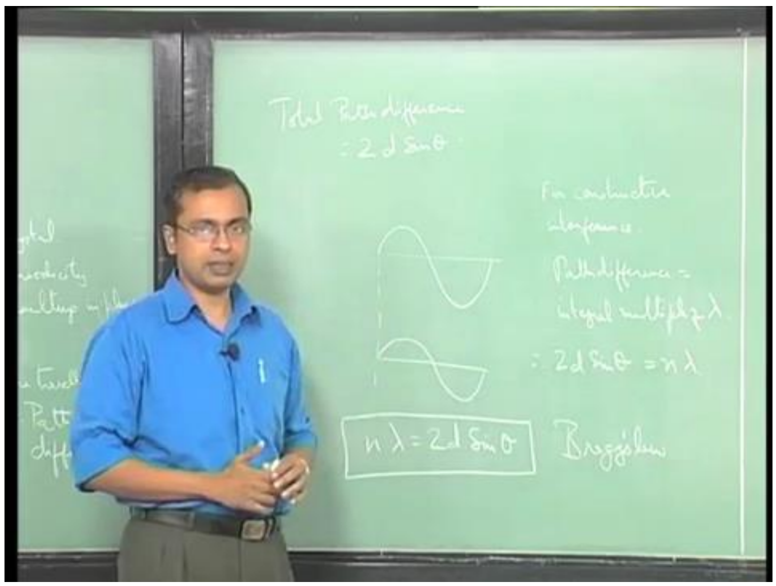

So, you can write that okay, so that is the total path difference between the two waves that have come to the adjacent planes and moved away from them. So that is the total path difference between there, so that is the total path difference. For constructive interference between those two waves that we are looking at, this path difference should be an integral multiple of the wavelength. Only then so for example you have a wave like this.

The wave from the adjacent plane could have travelled any amount of additional distance, but eventually when it comes to this point it should once again come back the same way. Then these two are exactly in phase, there is constructive interference. If it is not in phase then it is not going to be in constructive interference. So therefore whatever additional distance it has travelled eventually.

When it comes back here it should add up to an integral multiple of that the extra path that it has travelled should be an integral multiple of wavelength. Only then when it comes back to this location they will again be exactly in phase okay. If it is off by any, if it is 1., if it is 7.1 wavelengths then it is not going to be in phase, it has to be 7 wavelengths, just for an example right.

So, this has therefore got to be, for constructive interference a path difference should be equal to integral multiples of lambda. Therefore, we say 2d sine theta which is the path difference, total path difference should equal some integer n times lambda. When this is true, constructive interference occurs okay. So, n lambda or we just writing it the other way n lambda = 2d sine theta, this is the Bragg law, Bragg's law right, attributed to Bragg.

So, n lambda is to 2d sine theta, so this is the Bragg's law, this is derived, the concept behind its derivation is valid is in fact we are going to use the essentially the same kind of approach even when we look at the reciprocal lattice representation of this interaction. But this is, the way it is derived, it is derived in real space, we are looking at real space planes and the interaction of waves as they interact with those real space planes.

When they come off of those planes, how is it that they are constructively interfering? How is it that the interfering? And when they interfere what is the rule that has to be true for the interference to be constructive and so that is how we end up with this n lambda being here okay. So this is Bragg's law it is derived with respect to real space and in fact lot of the interaction between the waves and the periodic structure.

And therefore, for a lot of diffraction related experiments this is all you that is really required it does satisfy most of the information. However, there are subtle features of the diffraction process which this law will not be able to clearly indicate okay. So and for that the reciprocal lattice notation that we have the reciprocal lattice notation the reciprocal lattice method of telling us how and when diffraction will occur?

Is considered a much more robust way at much more fundamental way of describing the diffraction process and therefore is able to explain a lot more of the experiments that we encounter in diffraction lot more of the diffraction phenomena okay. So, but in real space this is the condition for diffraction to occur in real space right. So, this is the condition we will now look at the same diffraction process as it is laid out in reciprocal space.

And see whether see what is it that, we can understand from the process okay. As far as I will also say at this point that you know, as far as the actual diffraction process is concerned you have a periodic lattice, you have a wave they just interact and you see diffraction. So that is all there is to it in the real sense in the in terms of what is actually happening. Whether we describe it using real space notation or reciprocal lattice notation is simply a question of our convenience okay.

So that is all there is to it, so it is not that we are stating something different when we go into reciprocal lattice notation or we have changed the interaction in some way that is not the case. It is simply a manner of describing the interaction okay. So therefore, fundamentally things cannot change from what we have just described. Fundamentally what is happening is the same thing that there is a path difference between waves.

And whether or not the path difference adds up to some integral multiple of wavelength is all that we are looking at okay. So that is something we have to keep in mind. Even though we would look at some other description for it okay so we will do that.

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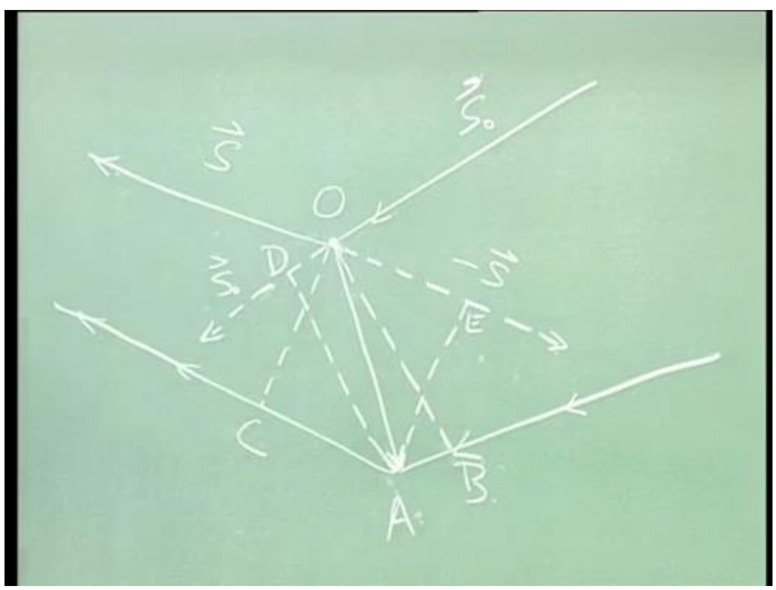

So now let us take up an atom at the origin O and some other atom at the location A right. So, we have two atoms here, which belong to this periodic crystalline structure. So, we have an atom at O and an atom at A, therefore this vector OA okay. Since this is a real lattice vector okay, so this is a real lattice vector. So OA is going to be, so we will say that, we will just described it as p times a1 + q times a2 + r times a3.

Where a1, a2 and a3 are the unit vectors in the real space okay, in real space a1, a2 and a3 are the unit vectors and p, q and r are integers and the reason they are integers is because that is the way we are defining the crystal structure. We define it so that when you have atomic spacing's you reach those atomic spacing or that is the lattice points.

You reach those lattice points based on integral multiples of a1, a2 and a3, that is how a1, a2 and a3 are defined mainly for our convenience. So, in terms of the standard convention used for describing lattice vectors and such p, q and r would be integers okay. So that we just need to keep that in mind. So, by definition we are saying this vector here is pa1 + qa2 + ra3.

Where p, q and r are integers because that would lead us from one that is point to another lattice point by based on a convention, so now we have again a similar situation we will say that a beam comes and strikes this atom and then goes off in some direction okay. So, we have this, so a parallel to this we have another beam striking this atom.

And it goes off in this direction or at least we are looking at we are going to examine this interaction of the same beam with this other point when it comes off in this direction. So, this is what we are planning to do. So now we look at some vectorial notation, we will say that this is the incident beam direction this is the diffracted beam direction okay. So, this is the incident beam direction this is the diffracted beam direction.

We will define a unit vector in this direction and a unit vector in this direction okay. So it is only a unit vector, it is not okay, so please keep that in mind. So, it is a modulus is unity, so we will say this is S0, S0 is the unit vector in this direction and S is the unit vector in this direction. So, these are unit vectors fine.

Now I will extend this or okay we can we can extend that in just a moment and we will look at the path difference now. So, this is going to be true even for these two waves because it is just unit vector, so this is also going to be in the same direction, so if this is also going to be S0, this is also going to be S as far as the unit vector direction is concerned okay. So now what is the path difference, so same thing we will do?

We will just draw a line which is which is perpendicular to this wave and see where it comes and touches this wave okay. So, I will call this B, so that is the additional distance this wave has travelled. Similarly, here we have to draw a perpendicular and that will be the additional distance travelled by this wave. So, we will do that ABC, so we have now.

So, path difference is, since we are looking at it vectorially, we will make sure that we are using the correct directions this is BA + AC okay. So, BA + AC, we can say, so or we want only the modulus at this stage. So anyway, we would say BA + AC that is the additional distance that is being travelled by this second wave okay. So, wave travels BA + AC that is what is being travelled.

Now what we will do is, we will actually for our convenience of calculation we will define both of them with respect to S0 and S. So, to do that more easily we will just extend this backwards, if I extend this line backwards, the opposite direction this is the origin right. So, the opposite direction here is -S okay. So, this is vectorial notation, so this is +S direction this is origin, I am going the opposite direction here.

So, this is -S fine. If I extend this line forward, this is in the same direction as the S0, I have not changed the direction, I am coming and I am continuing the same direction right with respect to the origin, with respect to the origin I am continuing the same direction and so this is still S0 okay. So now what I will do I simply look at this direction AB along this, so to do that I have just draw a line parallel to this starting from here.

So that will just come out to something like this. So, I am just transferring this distance onto this vector here, so that I can designate it with respect to that vector, that is what I am doing. It is still the same distance. So, A, B and C is already taken here, so we call this D and similarly this distance we will transfer onto here, so that we can take it with respect to S, -S okay.

So, this is now this is A, B, C, D, E right, so the same path difference BA + AC, now BA is simply OD they are both the same B to A is the same as O to D. So, this is equal to OD and AC is here A to C it is the same as E to O right. So, BA is OD and AC is EO, so therefore the path difference is simply EO + OD, the same thing. So, this is the path difference, this vector A fine, OA if you look at the, what OD is, it is simply the, is the component of OA along this direction.

So, there is some angle theta here, so OA cos theta is what OD is right, OA cos theta is what OD is some other theta is, I mean this is also theta here, OA cos theta would that, theta here would give us this value OE. So, in other words it is the component of OD is the component of this OA along this direction, along the S0 direction and OE is the component of the OA vector along the - S direction.

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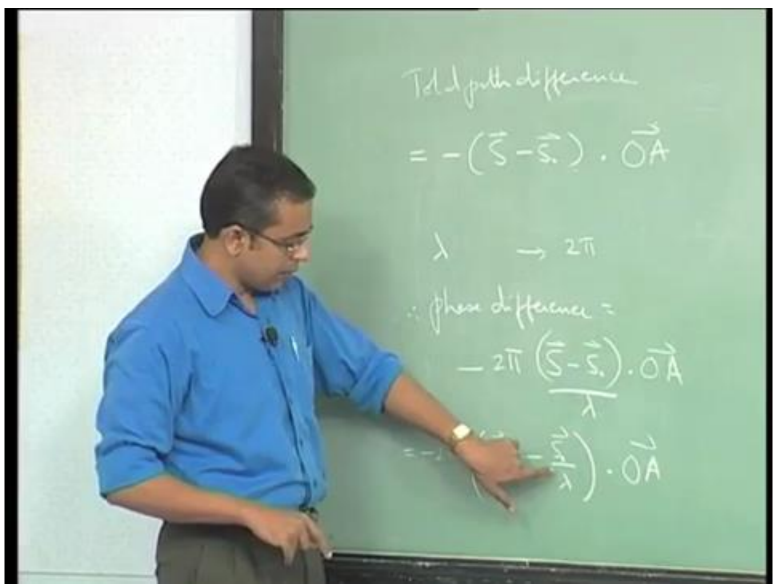

So, path difference is in fact just by convention it is written, we had a S0 –S, I will simply write it as - of S -S0, simply by convention it is written this way dot OA okay, so this is what we have. Now we basically say that you know a path difference of lambda is a phase difference of 2pi, so to get this path difference we are simply going to have, therefore the phase difference is = -2pi into okay.

So – S – S0 so simply, so this quantity times this, by this is the phase difference. So, it is just a proportional, matter of proportions. So, a path difference of lambda gives us a phase difference of 2pi. Therefore, a path difference of this gives us this phase difference. This path difference times 2pi divided by lambda. So that is what we have this path difference times 2pi divided by lambda, so that is the phase difference.

Now we already see this is a unit vector in the direction of the incident wave, this is I am sorry this is a unit vector in the direction of the incident wave. This is a unit vector in the direction of the diffracted wave. They are both divided by lambda, so we already have the 1 by lambda, 1 by length quantity beginning to appear here right.

So, what we will say is, we can in fact write this more specifically as - 2pi S bar by lambda -S0 by lambda okay. So, what we will we need to keep in mind is that this S0 by lambda, this S0 is the direction of the incident wave and 1 by lambda is the magnitude of it in reciprocal space, if you want to put it inverse space.

We need not worry about that in a specific way except that we need to understand this is a direction and the quantity here is 1 by lambda, so it is in reciprocal length quantity okay. So, in other words this vector is a reciprocal lattice vector. In reciprocal lattice vector 1 by length quantities are being portrayed okay and directions are portrayed. We now have a direction plus a magnitude of 1 by length.

Therefore, this is a reciprocal lattice vector or in other words it is ready to be represented in reciprocal lattice. You can directly represent it in the reciprocal lattice because it has all those attributes. It has got the 1 by length convention associated with it and it has a direction. So, it is a reciprocal valid reciprocal we will not say it is, it can be represented in reciprocal space.

When you say it is a valid reciprocal lattice vector it has to end at a reciprocal lattice point okay. So right now, we have not yet placed that restriction on this vector okay. So, and when I get to the, in a couple of steps I will reemphasize what I mean by that. Right now, it is simply it has got all the attributes to be represented in reciprocal space okay.

So that is the first thing we will note here. Same thing is true here, this is also a direction and this is 1 by lambda okay. So, in terms of the magnitude, in terms of its dimensions it is correct for a reciprocal space representation because it has got both the direction as well as 1 by length designation. So, in reciprocal space, so this is a vector in reciprocal space.

This is a vector in reciprocal space right. So therefore, this difference between these two vectors is also going to be a vector in reciprocal space fine.

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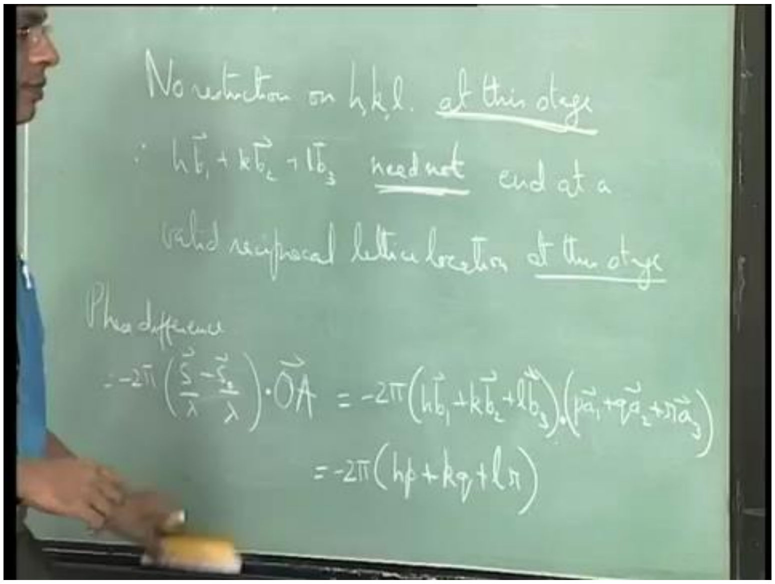

So right now, therefore we can what we can say is okay. So, this can be represented in reciprocal space that is all we say because it has got all the attributes to fit into reciprocal space. Now there is a very important point that we need to note here b1, b2 and b3 are reciprocal unit vectors in reciprocal lattice, in reciprocal space or unit vectors in reciprocal space, corresponding to the a1, a2 and a3 which we use to define OA.

The difference when we position two atoms at one atom at O and one atom at A, we used real lattice vectors a1, a2 and a3. Those are real lattice vectors defined for that real lattice unit vectors define for that particular lattice okay. So, they have specific magnitudes and directions using that were able to decide on the distance OA as pa1+qa2+ ra3 where p, q and r where integers.

Because that moved us from a lattice point which was O to another valid lattice point which was A fine. So those were two valid lattice points therefore OA was a valid real lattice vector okay. So therefore, that is the reason why p q and r had to be integers because that is the way in which we define such lattices.

We define them so that when you use integer movements of a1, a2 and a3, you will move from one lattice point to another lattice point. That is the way we define that right. So that is why p, q and r where valid where integers okay. So, and a1, a2 and a3 are the unit vectors in real space. Now corresponding to those unit vectors, we can define b1, b2 and b3 as the corresponding unit vectors in reciprocal space okay.

So that is what this b1, b2 and b3 are all right, now having said that the same logic holds in reciprocal space, in reciprocal space also if you start at the origin, if you move through integer multiples of b1, b2 and b3. You will arrive at a valid reciprocal lattice point okay. In reciprocal space, as in real space there are specific points which are valid lattice points okay. So, that those are the points that define the lattice.

The rest of the space in between does not really, is just empty space so to speak fine. So, if you do not move through integer values, you will reach some open location where there is no atom available or there is no lattice point available fine. So that is the point you have to understand, so in other words when you simply have b1, b2 and b3 you can multiply them by integers or you can multiply them by non-integers also okay.

So, you can multiply them by fractions. If you multiply them by fractions you will arrive at some non-valid lattice point, you will be in some open location where there is no lattice point. If you multiply them by integers you will arrive at a lattice point. So, the same is true for a1, a2 and a3 as it is true for b1, b2 and b3. You have to multiply them by integers to arrive at a lattice point, if you multiply them with non-integers you will arrive at some open location in general okay.

So right now, when we know, when we wrote pa1 + qa2 + ra3 because we moved from one valid lattice point to another valid lattice point p, q and r had to be integers. At the moment, the way we have defined this vector, we have not said anything about this, we have not placed any requirement that this has to be at a valid lattice point okay. So, at the moment it is simply the difference between two vectors in reciprocal space.

And these two vectors, we have not placed any restriction on them these two vectors are based on a beam that we have sent from outside. We have taken a sample a beam of x-rays for example or an if you are working with, let us say with an electron microscope of beam of electrons arrived at that sample and headed off in some direction for some interaction. So that beam is kind of independent of the sample that you have put right.

So, the direction in which that beam can be, the wavelength with which that beam comes is completely at your discretion okay or the instruments discussion. So therefore, this S could have been anything, this S0 could have been anything. Similarly, this lambda could have been anything. So, you have full freedom to select all of these three quantities which is what this left-hand side of this equation is.

Since you have full freedom to select anything, which satisfies I mean for the left-hand side of this equation. It therefore means that at the moment h1k, I mean h, k and l can also be any arbitrary number. It could be an integer, it could be a fraction, it could be one of them could be a fraction anything could be true right. So therefore, at the movement the way it is written even though we have used h, k and l no restriction is actually being placed on the values of h, k and l.

They could be any absolutely anything they could be integers, they could be fractions, any number that you can think of you can place here. So, no restriction has been placed on h, k and l, so at this stage of our definite definition no restriction has been placed on h,k,l. Therefore hk1, I am sorry hb1 + kb2 + lb3 need not okay. So, at this stage in our derivation, at this stage of in our derivation is what we are looking at.

We have not placed any other restrictions on the system. So therefore, this difference even though it has all the dimensions of being in reciprocal space. And therefore, can be written this way, it need not end at a, there is no, these h, k and l need not be integers and therefore this sum here which is now a vector need not end at a valid reciprocal lattice point, it could end up in some open location where there is no valid reciprocal lattice point.

So that is the important thing, now we are saying that the phase difference is = - 2pi in S -S0 by lambda or S - okay. So, this is what our phase differences is, therefore this is = - 2pi this is S by lambda -S0 by lambda is what this quantity is, so therefore we can write that by as that vector there hb1 + kb2 + lb3 right and OA we have already defined as pa1 + qa2 + ra3 and this is a dot product okay.

Dot product of hb1, kb2, lb3 dot product with pa1, qa2, ra3 where p, q and r have to be integers at the moment h, k and l could be anything they need not be integers, so if you do take the dot product so this is = -2pi hp + kq + lr. This is what we get; of which p, q and r are integers h, k and l could be anything. Now for constructive interference okay, so we have this phase difference, for constructive interference this has to be such that the path difference.

This phase difference should be integral multiple of 2pi okay. When we say integral multiple of wavelength, a wavelength is 2pi in terms of phase. So, if this becomes an integral multiple of 2pi, we have constructive interference because that means the two waves are exactly in phase okay. So, one may have travelled several additional wavelengths but at the end of it all they are both exactly in phase. So, for constructive interference this complete quantity here should be an integral multiple of 2pi okay.

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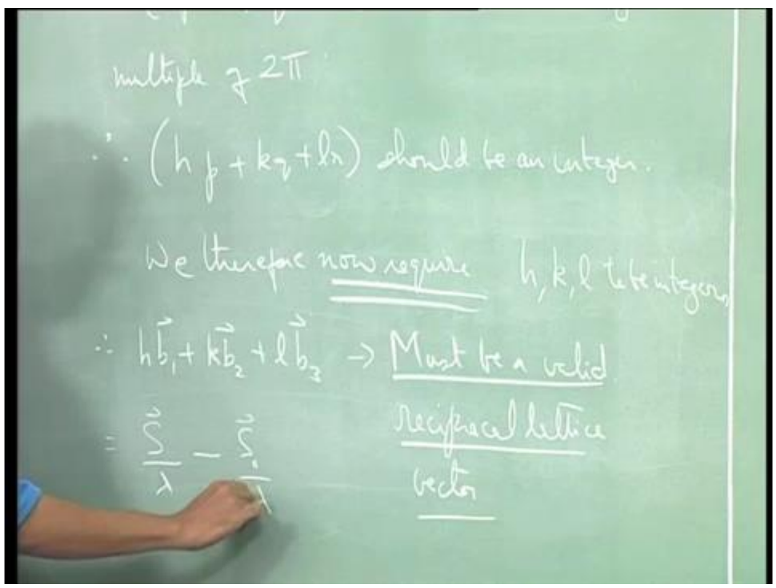

So, it has to be an integral multiple of 2pi, this is the phase difference this whole quantity is a phase difference that has to be an integral multiple of 2pi for constructive interference. We already have 2pi here, it therefore it means, therefore we are in, we are requiring that hp + kq + lr should be an integer okay. So, while we, when we first defined the S by lambda -S0 by lambda, we define that to be hb1 + kb2 + l b3.

But we place no restrictions on the values of hkl at that stage. However, we find that we are forced to deal with the situation for were in for constructive interference to occur a product some of these terms hp + kq + lr should be an integer in this p, q and r are already integers okay and they could be any integer. So therefore, for this complete sum to be an integer regardless of the values of p, q and r.

We now require, we therefore, we now require right h,k,l to be integers right. So, we therefore now require h, k and l to be integers. In our derivation, we find that we have reached a stage where originally were at a stage where h, k, l could have been anything. But the conditions we are placing on those interference processes.

The conditions, that the interference places on the set of relationships creates a situation where the h, k and l arrive at this particular sum where they are multiplied by p, q and r respectively. Where p, q and r were integers and that sum should be an integer, for this to be true regardless of the values of p, q and r, we can guarantee this to be true only if h, k and l are also integers okay.

So therefore, we now arrive at a situation where h, k and l which could have been anything earlier on, now have to be integers for constructive interference to occur. Therefore having reached the stage we are able to say therefore hb1 + kb2 + lb3 must be a valid vector, a valid reciprocal lattice vector okay. So therefore hb1 – kb2, I am sorry hb1 + kb2 + lb3 must be a valid reciprocal lattice vector. So therefore, we find and this is what, this is simply S by lambda – S0 by lambda okay, so this is what it is.

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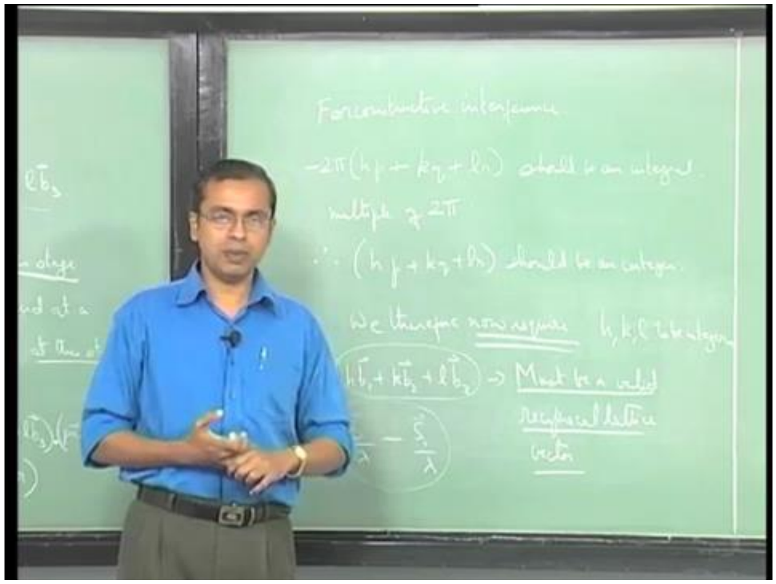

So, if you look at these quantities, the way it will work out is we need this difference to end up at a reciprocal lattice location okay. So therefore fine, so they should arrive at a reciprocal lattice location for constructive interference to occur. So, what we see is if you look at our equation here, we find that we have two different quantities here, we have a quantity on the on this side of the equation.

Which basically gives us all the properties of the waves arriving at the lattice arriving or leaving the lattice this is the direction in which the incident wave is arriving S0 and 1 by lambda is the magnitude of that wave in reciprocal quantities okay, magnitude of the wave in reciprocal quantities of the wavelength in reciprocal quantities. So, that is gives us the properties of the incident beam.

This is the properties of the diffracted beam this is the direction of the diffracted beam S and 1 by lambda is the wavelength of that diffracted beam in the reciprocal lattice, in the reciprocal space dimensions okay. So, this gives us all the properties of the incident beam as well as the diffracted beam in the reciprocal space notation fine.

So, all of the wave information is here, regardless of where the wave came from or what is the origin of the wave? That is irrelevant to us. All the wave information is here, what is up here on the other side of the equation has a valid reciprocal lattice vector okay. So, it is a line that is connecting to valid reciprocal lattice points.

So, this has got the crystal structure information in it. This has got all the crystal structure information in it, denoted in the reciprocal space notation right. So, we find that this equation okay, this equation here hb1+kb2 +lb3 = S by lambda -S0 by lambda that equation gives us the condition for diffraction as indicated in the reciprocal lattice, in the reciprocal space notation.

We have the reciprocal lattice vector representing information about the reciprocal lattice on one side of the equation. We have the reciprocal of the wavelengths with the directions indicating the wave information on the other side and the equation of these, the fact that they are equal to each other with h, k and l being integers and therefore being about a valid reciprocal lattice point.

Gives us the complete picture of how we would represent the condition for diffraction in reciprocal space okay. So, this is a, so this is the important derivation here fine. So, it has all the information that we require in terms of the both the reciprocal lattice crystals, so in terms of the crystal structure on one side, in terms of the wave information on the other side and taken together it is the diffraction information, diffraction condition.

So, we have derived today the diffraction condition both in real space as well as in reciprocal space. In both cases we have the structure information on one side and the diffraction condition on the other side. So, the diffraction condition we have derived in both formats the real space and the reciprocal space.