Introduction to Reciprocal Space

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Lecture -01
Reciprocal Space; Definition and Properties

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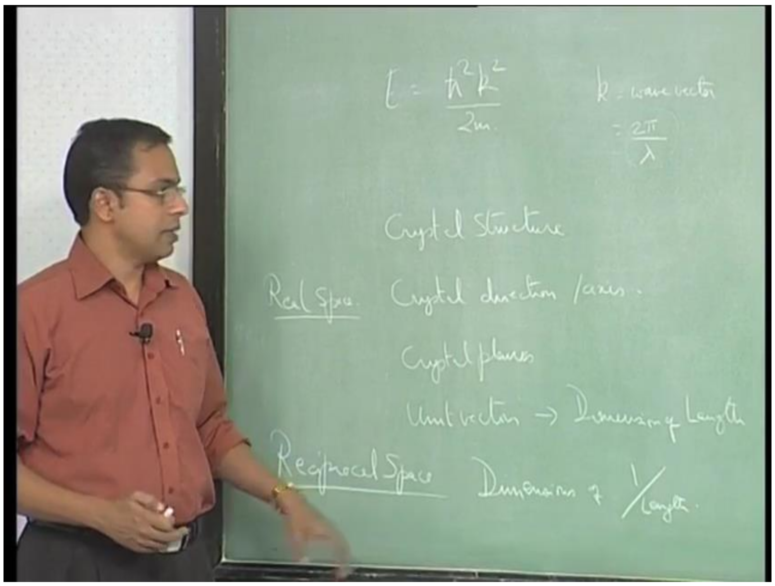

The crystal structure is something that you know in fact you have probably learnt off from high school days and certainly maybe early college days you have heard of crystal structure you have heard a lot of descriptions of it and so on. So, in those descriptions you would have heard of crystal directions in other words axis and crystal planes. So, there are conventions based on which we designate the directions and planes and so on.

And on that basis, you can have lot of the crystal structures that we have in the books okay. So, these are there normally these are in dimensions of length. We basically a certainly crystal axis when we unit vectors we say with respect to, so we define unit vectors dimensions of length okay. So, this is how it is done, we write xyz coordinate system we say you know and if you take a real crystal structure you may have specific dimensions.

In the form of say of the order of say 2 angstroms inter atomic spacing is of the order of 2 angstroms say 1.5 angstroms, 1.8 angstroms, angstroms is 10 power -10 meters, so it is still in the dimensions of length okay. So, when you normally put such information together okay, so we would call this as real space. A real space is what we are conventionally used to which where we write an xyz coordinate system.

And within the framework of that xyz coordinate system, we define dimensions, we define unit vectors, we define directions, we define the planes and spacing between planes and so on. So, this is real space okay, what we are going to do today is define something that we will call reciprocal space. You will define something called reciprocal space and we will begin to see some of it is properties okay.

Reciprocal space in fact takes the basic approach here is that the same crystal structure information that you have here or and many of its important key features can be represented in another format known as reciprocal space okay. So, we are not actually changing anything in a fundamental sense, because you are still talking of the same material, you are still talking of the same kind of relationships between the planes between those materials.

The atoms between those present within the materials and so on. So, we are not fundamentally changing anything. All we are doing is we are representing the same information using a different set of a different framework. If you want to call it that it is a different framework which is called reciprocal space, here the dimensions of the vectors we will use will be 1 by length. So, dimensions used to be 1 by length or length power -1 is the dimension that we will use.

In sort of a trivial sense you can see that this can be related to our k vector because k vector is already in the dimension of 1 by length okay. So therefore, it maybe it may make it easier for us to relate certain things associated with the wave vectors of electrons which are running across the crystal structure. To the crystal structure itself okay, if you use the same framework within which you are describing both of them.

The framework here we are using is 1 by length 1 by lambda. So, it would help, if we also define the crystal structure in 1 by length dimensions okay. So that is maybe a little bit of a trivial way of saying it, but it will it is it certainly conveys the immediate link between what we have just done up until now and what we are planning to do okay. In reality, actually it is much more than that it turns out that many of the information.

You can represent in 1 by length in this reciprocal space. Actually, conveys certain details of how interactions occur between a crystal structure and waves that are present much more elegantly. Then is done in real space okay, so in a broader sense this is, this conveys certain information much more elegantly reciprocal space and actually is able to highlight specific details a much better than the real space way of representing information does.

And that is the real, that is the fundamental reason why actually if you get into diffraction. If you get into I mean diffraction as a means, as a tools of, as a tool for looking at structure and such information characterization of materials. You will find a lot of heavy usage of reciprocal space.
The first time we encounter reciprocal space it is not as intuitive and it may seem like you know we are unnecessarily complicating the issue so to speak okay.

So, it looked like why go to all the troubles of creating everything in 1 by length when real space is already there for us. It is just that if you use it enough you find that there is lot of information that is much more elegantly and clearly represented in, when you use this notation than when you use real space notation.
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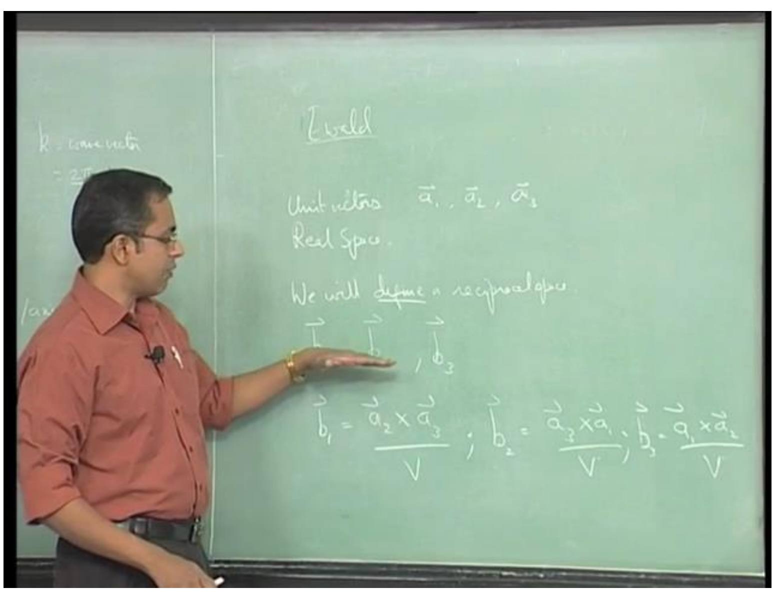

So, it is from that perspective that this is really caught on and it traces itself back to a person by name Ewald, who actually worked on this in around the year 1920 okay. So around that time frame was when this work was put together. And so, there is a notation which is which is named after him also in this relationship okay, so in this context. So, we will see that as I mentioned you know we have sort of indicated why you may need to go in for 1 by length dimensions.

But that is not a hard and fast, that is not the best way of indicating, but you can see the link that we have already got 2pi by lambda for k wave vector and we want to see the interaction between the electron waves and the crystal structure and therefore it would help if we or if you present at all the information in the same framework. So, you can think of that as a loose link for what why we are doing what we are doing.

As we progress forward we will see much more a better understanding of how this system works out okay. So now we will look at in the next 2 or 3 classes we will actually focus exclusively on reciprocal space and we will build its relationship to the real space because that is something we need to understand. And to some degree this discussion may seem a little disconnected from what it is that we have discussed so far.

But we will need to build this framework, so that we can connect it up link it up to our discussion earlier and see what benefits we can gain from the process okay. So, but temporarily for at least this class and in most of next class this will be a discussion exclusively on reciprocal lattice and on how diffraction can as a phenomenon can occur in the reciprocal lattice. After that only we will make a link back to real lattice, a real space.

And also take up in extend this idea the diffraction occurs in reciprocal space and it has a certain way of being conveyed and see what is the consequence of that discussion, on how the electrons are interacting with a crystal lattice. So that that step is going to be 2 or that is at least 2 classes away before we get there. But now we will have to build the framework which will enable us to handle that discussion ok so that is what we would do at this point.

So, when you look at real lattice real space, we say that you know we are usually defining it by unit vectors and typically we would use the notation a1, a2 and a3 okay. So a1, a2 and a3 are unit vectors in real space. So, we have a crystal structure in real space represented by these unit vectors a1, a2 and a3 okay. Now we will define a reciprocal space in other words, we will define a space, we will define a coordinate system.

So, we are just going to define it up front this definition is at this stage may look somewhat arbitrary, we will just accept it as an arbitrary definition. The definition the way it is given will give the space a lot of useful properties which we can use later on. How arbitrary or otherwise this definition is we will see a little later but at the moment it is just a definition we will just accept the definition and we will work with it, so we are defining it okay.

So, this is a choice we are making, so we are defining it we are defining a reciprocal space to consist of three vectors again unit vectors there b1, b2 and b3 but these are not arbitrary vectors they are being defined with respect to real, I mean real space vectors in a certain way in other words there is in the process of this definition we are already making a link between these vectors and these vectors okay and what is that link it is written like this. So b1 is a2 cross a3 by V.

What this V is we will see in just a moment. It is a volume actually volume of this unit cell of consisting of a1, a2 and a3, b2 is defined as a3 cross a1 by V and b3 is similarly is a1 cross a2 by V. So, these are cross product, these are vector cross products so that is what they are, so these are all vector quantities b1, b2 and b3 are vector quantities. So, they have a magnitude as well as a direction, a1, a2, a3 are also vector quantities they all also have magnitude and direction and this is a cross product.

And so, it is defined that way b1 is defined as a2 cross a3 by V, b2 is defined as a3 cross a1 by V and b3 is defined as a1 cross a2 by V okay. So, this is the way they are defined. By defining it like this certain properties become, certain properties arrive for; I mean end up being available for b1, b2 and b3 which becomes convenient for our utilization later on okay. So now we will see what immediately based on this definition itself.

Simply because we have defined it like this, what is the meaning of what is the consequence or what is the relationship between b1 and this reciprocal, so these are called reciprocal lattice vectors okay. These are unit vectors in reciprocal space they are also called reciprocal lattice vectors. These are real lattice vectors and this is real space. So, by simply using this definition what is it that we have created as a relationship between. What is the consequence in the relationship between b1, b2 and b3 with respect to what we have in real space? So that is the first thing that we will examine okay.

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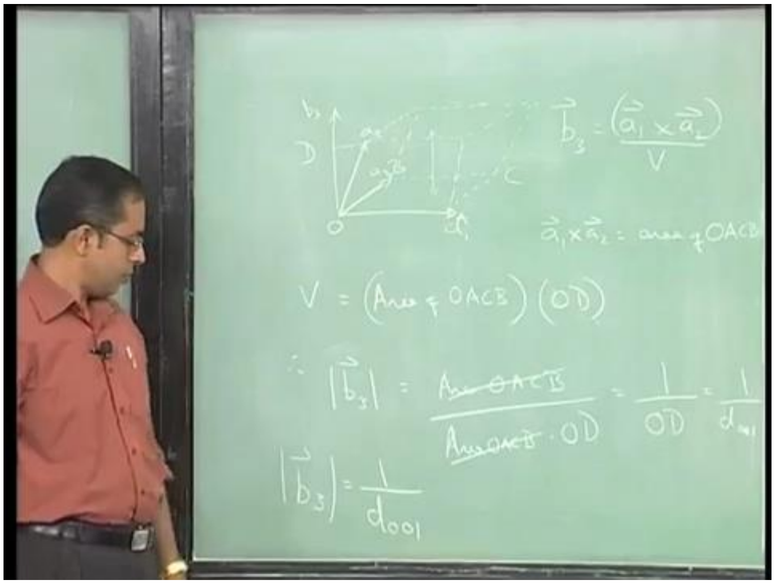

So, to do that let us take an arbitrary say a triclinic cell. A triclinic cell is one where by definition the a1, a2 and a3 vectors need not have the same length. So a1 need not be equal to a2 need not be equal to a3 and the angles between them, so alpha beta and gamma which are the three angles that exist in the system need not be the same okay. So, in that sense it is of it is like a very general cell.

We have placing a really placing no restrictions on it. Now we are defining we will write b3 again here fine, a1 cross a2 by V. So, now by definition see volume does not have any is not a vector, volume is just volume it is not a vector, it is a scalar quantity. So, you have a1 cross a2 by definition of cross product, if you have a cross product the result is perpendicular to both a1 and a2 okay.

So that is the meaning of a cross product. So, b3 therefore by definition is perpendicular to a1 and a2. So, on this scale if you want to draw b3 it will show up something like this. It will show up somewhere in this direction it would be perpendicular to the plane being described by a1 and a2 okay. So, the planes a1 and I mean the vectors a1 and a2 define a plane which we are now treating as the horizontal plane on this board a sort of in this representation.

And b3 would now appear in this direction perpendicular to a1 and a2. So that is the definition by way of definition. But what about its actual magnitude, if you look at a1 cross a2, if you see the by the standard definition of a1 cross a2 that is the area of this parallelogram okay. So, if you write this as the origin write this as OA, let us say this is B and let us say this is C, so the area of this parallelogram OACB is what is being given by a1 cross a2 okay.

So OACB area of parallel a1 cross a2 okay, OACB the parallelogram. So that is what this area is, if you look at the volume of the unit cell, this V here is the volume of the unit cell in real space okay. So that is the volume that is that V. So, which is that volume if you take this a3 vector and you complete this solid okay. So that solid, so this unit cell that we have drawn here I mean if you draw it properly you will get it appropriately.

This volume of this unit cell is this volume V that we have written here fine. So that is the volume that we are looking at. So, what is that volume in terms of geometrical terms it is simply the area of this base times the distance between these planes or the height of this unit cell okay. So that is all the volume is, the volume is the area of the base times the height of that structure. So that is what we are looking at.

So, the height is simply this the whatever, this is ABC so this is D let us call this D, OD. So, OD is the height of this unit cell that we have drawn and it is simply the projection of a3 on this axis. Which is perpendicular to a1 and a2 right, so that is the height, so we will call that so the height is OD okay, so the height is OD. So therefore, volume is the area of OACB into the height OD okay.

So, it is a product of the area times the height that is the volume okay. So therefore, if you look at it that way b3 okay or the modulus of b3, is area OACB by area OACB into OD. So that is what the modulus of b3 is, so these two will cancel out, so it is simply 1 by OD, so it is simply 1 by OD okay. So that is the magnitude of b3, so b3 is in this direction and the magnitude of b3 is simply 1 by OD.

What is 1 by OD? If you look at the conventional planes that we are looking at if you look at the way we define planes this is the 100-plane okay. So, if you look at 100 plane, this is a d11, d100 plane it is spacing between 100 planes. If you go back to your elementary crystallography the 100 planes are defined this way and then these are 001 planes, d001 this is perpendicular to a3 axis okay. So d001 if you want to call it 001.

It is the spacing between 001 planes, so spacing between 001 planes is what we have now looked at. So, OD is the spacing between 001 plane, so d001 okay, so b3 is therefore spacing. This is the standard notation for crystallography, so if you go and look up crystallographic from your elemental crystallography this is d001 is the spacing between 001 planes and modulus of b3 is simply 1 by d001 okay. So therefore, we find and by analogy in fact I mean.

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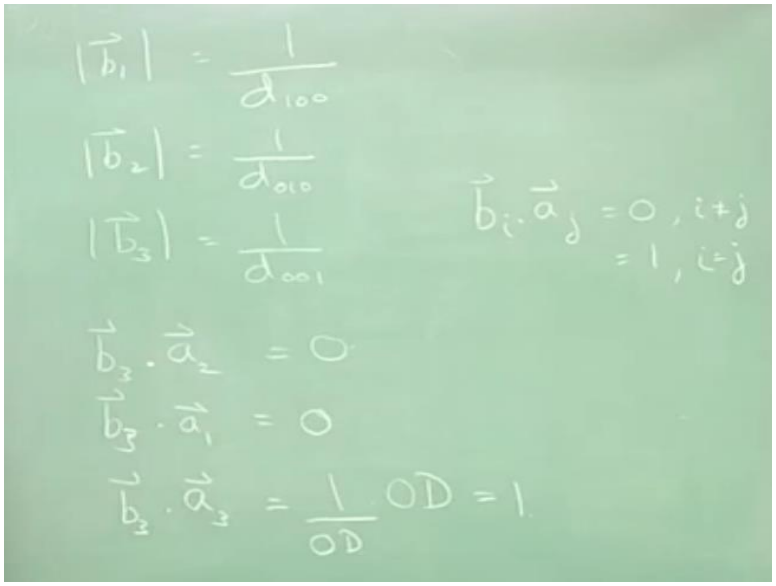

In fact, if you extend this argument the same thing would hold for the other ones too b1 is 1 by d100, b2 1 by d010 and b3 which we just did is 1 by d001. So b1, b2 and b3 are inversely proportional to the spacing of those planes 100, 010 and 001 planes. So that is the by way of our definition we have created the situation okay. So, it did not arbitrarily occur, since we defined it this way this is the way it has occurred okay.

Also, if you look at the way we have defined it, we will also see that if you just take a product say b3 cross a2 or b3 dot a2 okay. If you just take this dot product between b3 and a2, I have just arbitrarily pick these two vectors. We find that since b3 is already perpendicular to a1 and a2 this dot product is 0 okay. So, by definition it will be there will be a cos 90 degrees which was up here therefore this is 0. Similarly, b3 dot a3 sorry a1 equals 0.

Because b3 is perpendicular to both a2 and a1 simply based on how we have defined it that is all it is okay. So therefore, these two are 0, if you look at b3 dot a3 okay. Based on our definition if you go back to our the picture we have drawn here b3 has this distance OD, I am sorry this is 1 by the distance OD, so which we just saw here okay 1 by OD, b3 is modulus of b3 is 1 by OD, so this is simply equal to 1 by OD times the projection of a3 on b3 okay.

When you do a dot product that is basically what it is it is one vector times the projection of the other vector on itself okay? So, what is the projection of a3 on b3, projection of a3 on b3 is OD, a3 on b3 the projection of a3 on b3 is OD as shown in this diagram fine. So therefore, the dot O, dot a3 that we are having in that dot product is simply works out OD, so to speak. So, this projection will become OD okay.

So therefore, this is equal to 1. So, we find the relationships between those vectors the reciprocal lattice vectors and the real lattice vectors based on how we have defined those vectors okay. Based on how we have defined those vectors creates the situation where b3 dot a2 is 0, b3 dot a1 is 0 and b3 dot a3 is 1. So more generally if you have b i dot a j, then this is equal to zero, when i not equal to j and is equal to one, when i = j okay.

So that is the notation that we have and that is the consequence of what the wave in which we have defined these vectors okay. Now we have already seen, if you have taken a specific case actually, where we are saying that if you have a particular vector. So, b1 in this case is a particular vector and we found that the way we have defined it, it works out to be perpendicular to the two vectors a2 and a3. And it is equal to the, in magnitude it is equal to 1 by the spacing d100 okay. In reciprocal lattice, we can actually generalize this much more.

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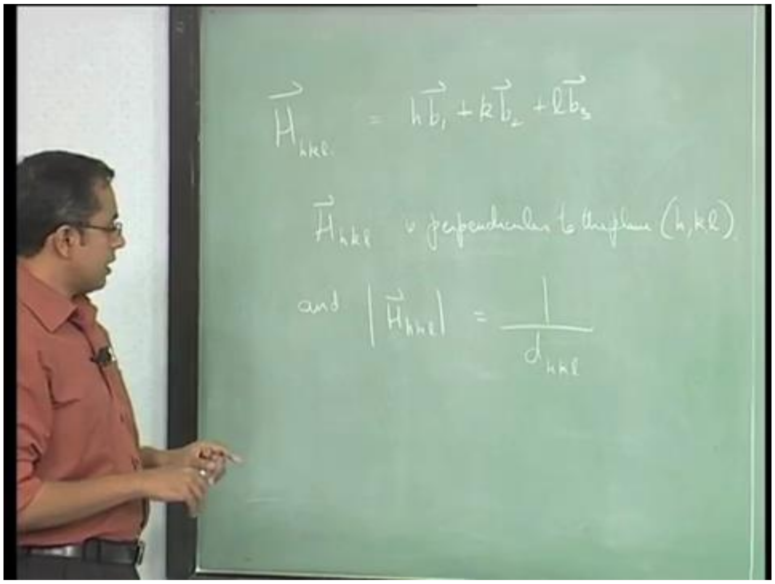

We will generalize it as follows; we can write any vector Hhkl, H is the notation that is given for a reciprocal a general, a generic reciprocal lattice vector okay. So, where we it could be anything, so H is a general reciprocal lattice vector, we will give it subscripts hkl okay. So, if this is a reciprocal lattice vector and the unit vectors in the reciprocal space are b1, b2 and b3 then this is simply equal to hb1 + kb2 + lb3.

This is simply based on our definition and vectorial, standard vectorial notation, standard vectorial notation b1, b2, b3 are unit vectors and h,k and l are the specific distances we are travelling along those unit vector directions okay. So Hhkl is a vector in reciprocal space and it is therefore equal to hb1+kb2+lb3, those hkl are the amounts that we are travelling on those respective dimensions okay so that is what it is.

We say that when we define, when unit when reciprocal space is defined the way we have just defined it, then when you take a general vector Hhkl okay, in the reciprocal space, we can there are some relationships it has to real space vectors and dimensions in real space just the way b1, b2, b3 themselves have relationships to the a1, a2 and a3 okay. We just saw a relationship between b1, b2, b3 and a1, a2, a3.

Similarly, we there is a very general relationship between any hkl vector in reciprocal space and certain quantities in real space. What is that relationship it is basically that Hhkl is perpendicular to the plane which has the Miller indices hkl and modulus of Hhkl = 1 by dhkl. Please note in both these cases we are relating something in reciprocal space to something in real space.

This is not complicated because we just did that already when we looked at a1, a2, a3 and b1, b2, b3 and we made relationships between them when I said that know b1 is 1 by d100, b2 is 1 by d 010 and b3 is 1 by d001 , there b3 is a reciprocal lattice quantity and d001 is a real lattice quantity. We found that you know it is simply because of the way we have defined it, when in our definition itself we have linked real space and reciprocal space.

So, they are not arbitrary quantities okay, so they are already linked by definition therefore some quantity in real space can relate to something in reciprocal space within the framework of the definition. So, that is basically all we are doing here this is a reciprocal lattice vector and it is found that it is perpendicular to a plane in the real lattice. Which has that the Miller indices h,k and l and the modulus of this reciprocal lattice vector is 1 by dhkl.

These are properties that the reciprocal or in other words one by the spacing of hkl planes. So, these are two properties that any vector in the reciprocal space has, as a result of the definition of the reciprocal lattice okay. So right now, I have just stated it in the next few minutes we will prove these two. Once we prove these two we have a good understanding of what holds in reciprocal space and how it relates to real space and later we can use those two okay.

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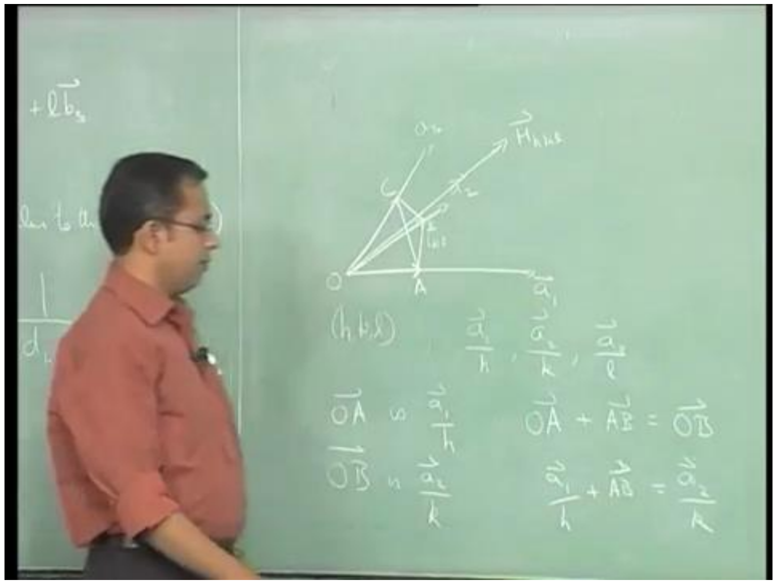

So, we will now try an attempt to prove this, so to do that let us actually draw a general plane in the real space. So, we will say that we have, so this is a1, this is a2, this is a3 okay, so these are unit vectors in real space and we will draw the hkl plane here okay. So, this is hkl plane fine, so now we will just say that in reciprocal space we have the Hhkl, we at this moment I am just arbitrarily denoting it here.

This is an arbitrary denotion at the moment, I have arbitrarily denoted it this way, I have indicated it here in this figure this way simply for the sake of convenience to show it in the same figure what relationship it actually has to Hhkl is not forced upon it simply because of how I have drawn it we will show that in fact it does have some appropriate relationship. So that relationship we will just see we are actually going to prove it.

Now by definition of hkl plane its intercept along a1, a2 and a3 are simply a1 by h, a2 by k and a3 by l. So, these are the intercepts okay, only because the plane hkl happens to intercept a1, a2 and a3 at those locations such that its intercepts are at a1 by h, a2 by k and a3 by l, that is the reason why we even call it the hkl plane okay. So therefore, if you see if you take this vector here, this vector here is a1 by h this is a1, a1 by h is this vector that is why you get this h notation in the hkl plane.

Similarly, this vector here will be a2 by k that is why you will get the k notation. This vector here from here to here is a3 by l that is why you get that l in the hkl. So, this is a1 by h. I will also name this locations where this plane intercepts a1, a2 and a3 as A, B and C okay. So, OA is a1 by h and OB, so this is origin O, OA, OB and OC. So, OA is a1 by h, OB is a2 by k fine, so this is what we have. So simply by vectorial notation if you write OA + AB you should get OB right.

So, OA simply because of standard vectorial notation, OA these are vectors by the way OA + AB should equal OB, that is easy to see, if you go from here to here and then you go from here to here, it is the same as going from here to here that is all it is OA + AB is OB. So, this is what we have a2 okay, so now that we know these are the vectors we can replace them OA is a1 by h and OB is a2 by k. So therefore, a1 by h + AB, vector AB should equal a2 by k fine. So, this is what we have, we can rearrange this a little bit.

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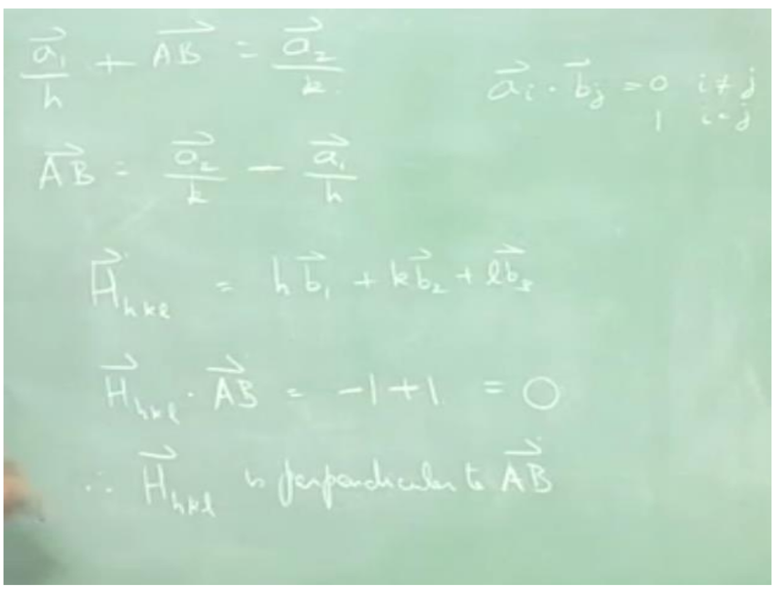

So, we wrote a1 by h + AB = a2 by k, rearranging this we get AB is a2 by k + sorry - a1 by h. So, we now have in terms of the a1, a2 vectors we have the vector AB given to us in terms of the unit vectors a1 and a2, which we have already defined for a real space. We already said that if you take a vector Hhkl, we are defining it based on this notation as hb1+kb2 +lb3. So, the hkl, h, k and l are simply integers okay.

So, this is some vector in reciprocal space, so h, k and L are just integers, so as long as they are just integers you can use them in whichever space you wish they are just integers, b_1, b_2 and b_3 are reciprocal lattice vectors. Therefore $hb_1+kb_2+lb_3$ is now a reciprocal lattice vector. Whereas, when you use the h, k and l which are just integers in the real space a_2 by k and a_1 by h, if you take this difference which is AB it is a real lattice vector.

Because these are just integers where which you are using in the real space, but they are the same integers at this time we have the same h k and l being used in two different places. The hkl plane is this results in this relationship and the same hkl values, we have now used for this definition although we have got no significance for it. Yet there is the same we are enforcing the same hkl in this definition for H_{hkl}.

So, if you now take a dot product of H_{hkl} and AB, what will you get? So, if you do H_{hkl} dot AB okay. So, we have b_1 here hb_1 okay, we already saw that if you have a_i dot b_j then this is equal to 0, if i is not equal to j and this is = 1, if i = j and since it is a dot product you can have at a_i dot b_j is the same as b_j dot a_i, if the order in which you do this dot product is not important to us because either way you will get the same thing.

So, if you look at this dot product here, you have hb_1, hb_1 dot a_2, so these are just the h is just an integer b_1 dot a_2 is zero because it is 1 and 2 here. So that is 0, b_1 dot a_1 is 1 and you have a hb_1 here and a_1 by h here so h and h will cancel you get -1 okay. So, hb_1 times or dot product of hb_1 and a_1 by h will give us - 1 right. If you take b_2 here kb_2 times a_2 by k, the k and k will cancel, you will have b_2 dot product of b_2 and a_2 which is 1 + 1.

And this b_2 dot a_1 is going to be 0 because it is a subscript 2 and that is a subscript 1 we already saw that by definition. So that is a plus 0, so that term will become 0 and then b_3, b_3 dot a_2 is going to be 0, b_3 dot a_1 is going to be zero. So, this term does not contribute in any way, it becomes all 0, so this becomes 0, so this becomes 0 the product with this gives us a +1 the dot product with this gives us a – 1, so this is equal to 0.

So, we have a situation where a vector in reciprocal space H_{hkl} dot vector in real space is equal to 0. So, in other words we have a dot product between two vectors which is zero, which simply implies that Hhkl is perpendicular to this vector AB. Therefore, Hhkl is perpendicular okay. So, if you go back to our figure it means that this Hhkl is perpendicular to this AB okay. So, this AB is there the way this Hhkl is defined it is perpendicular to AB.

Using exactly the same derivation that we have done instead of we started with this location being a1 by h and this being a2 by k. We can do the same thing with a2 by k and a3 by l okay, in which case we will find that Hhkl will become perpendicular to BC. Similarly, we can also do it with a3 by l and a1 by h and exactly the same calculations we will do we will find that Hhkl is perpendicular to AC.

So, we find that Hhkl is perpendicular to AB it is perpendicular to BC and it is perpendicular to CA, based on the same derivation that we have done. You simply have to select the other two axis, you will come to the exact same conclusion. The same math will, the mathematics is work out in exactly the same way we will find that Hhkl is perpendicular. The vector Hhkl is perpendicular to the vectors AB, BC and CA.

Therefore, and since all of these three are forming a plane, if it is perpendicular to any two in fact even if it is perpendicular to just two, it is certainly perpendicular to two and it is also perpendicular to all three. If it is perpendicular to them it is therefore perpendicular to the plane defined by A B and C okay.

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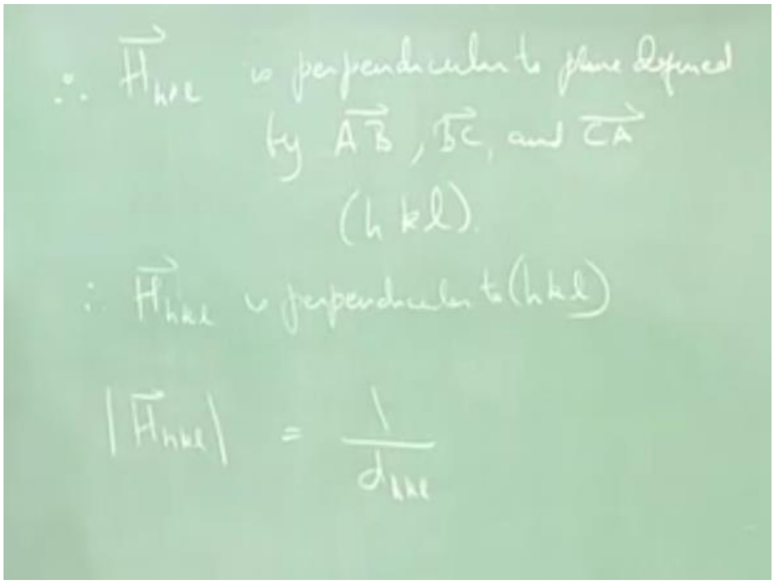

Therefore, Hhkl is perpendicular to plane defined by ABC, AB, BC and CA and therefore which is basically the Hh, which is basically the hkl plane okay. So that is how those vectors are even defined AB and BC and CA were defined based on the intercept at 1 by h, 1 by k and 1 by l in those respective axes. So therefore, Hhkl is perpendicular to hkl. So, any, so again we are relating something in reciprocal space a vector in reciprocal space to a plane in real space okay.

And again all these relations are coming about simply because our original definitions related a reciprocal lattice vector to real lattice vectors. So that relationship was already there within the framework of this relationship we are finding other relationships that hold. So, we find that any Hhkl plane which is that, therefore defined as hb1 + kb2 + lb3, where b1, b2 and b3 are the unit vectors and reciprocal lattice reciprocal space.

Those Hhkl vectors will automatically be perpendicular to the hkl planes in the real space okay, so this is already we have seen this. So, we have just we have just shown this okay. So, the other thing we would like to see is what is the value of modulus of Hhkl and how does this relate to the spacing of between the hkl planes. We will in fact see that this is equal to 1 by dhkl okay. So, this is what we are just about to we are going to look at.

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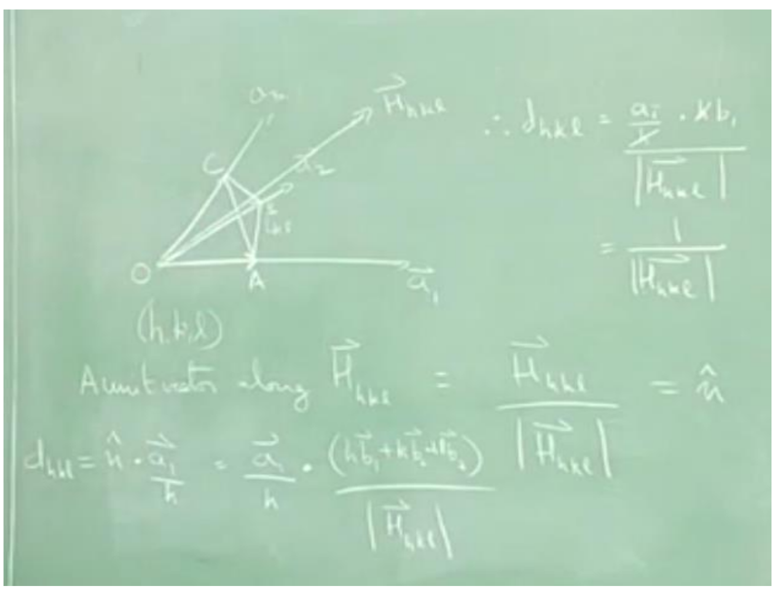

We will come back to this figure, let us say that a unit vector along Hhkl okay, so we will let us first define a unit vector along Hhkl that is simply Hhkl by modulus of hkl, of Hhkl right that is the definition of a unit vector along Hhkl. We will just call this say n, n cap okay. Now when you say a hkl plane is defined the way we have just drawn it okay. So, when we say this we mean that there is a similar plane like it at the origin.

Then there is one at this location, then there is one similarly spaced next to it, similarly space next to it and so on. That is the way we define a family of a set of planes. When you say a hkl plane it is not just a single plane I mean it is that set of planes that are parallel there. We take the one closest to the origin and then take the intercept of it and that is how we come up with Hhkl, so there are planes correspondingly apart.

So therefore, the spacing between the hkl planes is simply the distance between the origin and this hkl plane right. The closest distance or rather the perpendicular, the spacing between this origin and that location, which would then be the closest distance between the this plane and the origin is therefore the dhkl right. So now we have basically seen that the, at that point the line drawn from the origin.

Which goes closest to this plane will then they will then go perpendicular to that plane all right. So that is how you will get the location. So therefore, if you look at the distance between the plane and the origin, we basically see that we can write that by saying Hhkl or n cap dot a1 by h ok. If you take the dot product of a1 by h and you take it's, what shall I say the dot product of OA with this vector in the direction of this Hhkl.

Then you get the component of OA along that direction and that would then be the spacing that you are interested in okay. So, this is what you will get, so this is simply a1 by h dot product with you will have hb1 + kb2 + lb3 divided by the modulus of Hhkl okay. So, this is dhkl right, so dhkl is now defined this way d between those planes is such that the if you take the component of any of those intercepts along the perpendicular to that plane okay.

So that perpendicular is now going through the origin. So that perpendicular vector that is there if you take the component of this vector along the direction of the perpendicular, you therefore get the distance in this direction okay. So that vector unit vector is simply giving us the direction there but if you take the component of this intercept OA along that direction or any of this OB along the direction or OC along the direction.

If you take the component along the direction that would then represent that spacing between the origin and that point, which is then the closest spacing between the origin and that point and that would therefore and at that point that vector will be perpendicular to that plane, which is what how we have defined it okay. So, if you take the component of the intercept along the perpendicular that is the closest approach that the plane makes to the origin.

And that is therefore that d spacing of that plane because the next plane is sitting at the origin. So, the dhkl is the component of this vector a1 by h along this unit vector here. The unit vector is simply defined by this and this is and since it is a dot product we can interchange the, I does not matter which order we do it, so we will get this. So now if we carry out this dot product what do we see again you have an a1 here you have a b1, b2 and b3 here.

And clearly a1 dot b2 is 0 and a1 dot b3 is 0, the way we have already seen. So, only a1 dot b1 is going to count for anything else so okay. So a1 dot b1 is going to be 1 because of the way it is defined and the h and h is, are going to cancel. Therefore, dhkl is equal to a1, so we will just write it here, a1 by h dot hb1, b1 or sorry a1 dot h by hb1 dot hb1 divided by modulus of Hhkl. So, this and this will cancel a1 dot b1 equals 1 therefore this is equal to 1 by Hhkl here, so we see which is the proof, that, we wanted to be set out to prove.

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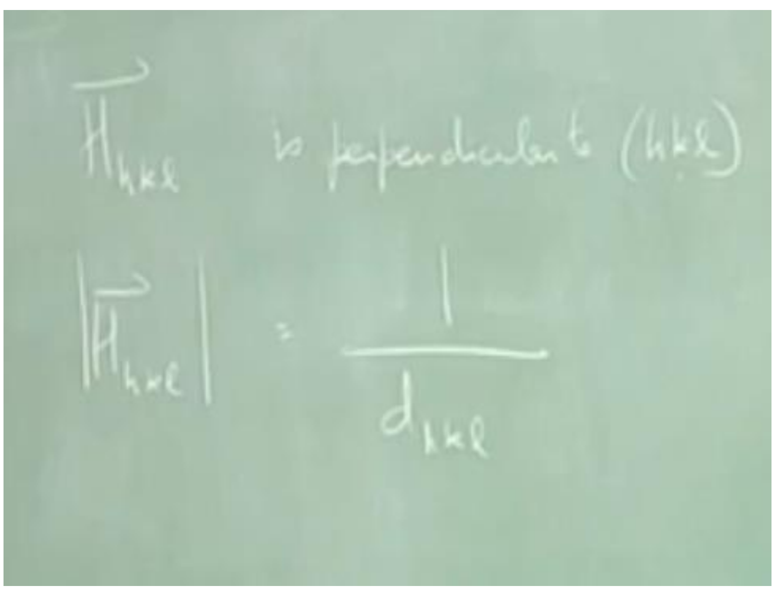

So, we see that Hhkl is perpendicular to and modulus of Hhkl is equal to 1 by dhkl okay. So, what we have seen is, we started off this class by saying that we need a notation or which is this reciprocal lattice notation. Because it will help us understand the interaction between the wave vectors corresponding to the electrons and the crystal structure which is basically conveys to us the periodic structure that is present between all the components that are present.

All the atomic components that are present within the lattice. So, to speak the material that we have so in that context we found, we indicated that basically we might need to develop something in this reciprocal lattice notation and it is that notation that will help us capture this interaction between the wave vectors and the periodic crystal structure.

So in that context we define reciprocal lattice to be consisting of b1, b2 and b3 with specific relationships to the real lattice vectors a1, a2 and a3. On the strength of that relationship we found that, on the strength of the definition we found that already b1, b2 and b3 had specific relations to a1, a2 and a3 which then translated to a general reciprocal lattice vector Hhkl having specific relationships to the plane hkl in real space.

The relationships are that the vector Hhkl is perpendicular to the plane hkl, reciprocal lattice vector perpendicular to a plane in real lattice. And the modulus of the reciprocal lattice vector is 1 by the spacing between those hkl planes okay. So, this is the framework of our reciprocal space we already seen some important relationships here.

In the next class, we will see how diffraction which is the interaction of waves with the periodic crystal structure. How the diffraction phenomena can be represented in the reciprocal lattice notation.