Physics of Materials
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Lecture No. # 27
Reciprocal Space – 1:
Introduction to Reciprocal space

Hello, welcome this is our twenty seventh class in this physics of materials course that we have begin going through these past several classes. So, we will sort of start where we left of last time, last time we actually realize that our Drude Sommerfeld model was actually pretty good, and both conceptually as well as in terms of the number that it gave us, it was able to show distinct improvements over the Drude model. Specifically, the specific heat constant volume, electronic contribution to specific heat at constant volume, which was a big issue with the Drude model was sorted out very well by the Drude Sommerfeld model.

We finished off last class by recognizing that the way those models have come about the Drude model, and the Drude Sommerfeld model, that is the initial version of the Drude Sommerfeld model, there is no input from the crystal structure into that model. So, in fact largely the structure of the solid is ignored, so one might of course ask the question so what, I mean we ignore the structure of the solid, how does it make a difference. The and to what extent is it justified or to what extent is there are problem with that kind of a approach. The issue is simply this, if as we highlighted in the end of last class, if you look at experimental values of several parameters that you can look at including conductivity say thermal conductivity, electronic conductivity certainly.

We find that in most materials there is significant anisotropy, this potential for significant anisotropy and there is significant isotropy in some materials, in the value of the property based on the direction in which you are measuring it. So, there is significant variation, and therefore anisotropy. So now, if you are simply looking at it from the perspective of number of free electrons per unit volume, that is going to be the same regardless, because that is that is a quantity that is defined irrespective of direction right. So, it is a it is defined as the same value irrespective of direction.

So, if we define the property only with respect to that are we carry out all our calculations only with respect to that, without any wave shape or form taking into account the structure of the solid, then somewhere we loose the link between the two of them. And and are at least we should end up with the same value regardless to the direction. So, the only thing in the in the solid, that represents strong directionality of the solid is it is crystal structure, so that is the first important point that we have to keep in mind.

So therefore, in our models, in the as we go about improving our models, we have to somehow incorporate the crystal structure into the model to understand and to incorporate the interaction of these electrons with that crystal structure, so that is clearly a step we have to take and may be at that stage we can reassess to see if we have, if the picture we have produced is now meeting most of the criteria, most of the parameters that we are able to measure experimentally. And it turns out that in fact if we do it, we are we are pretty much there in terms of having a fairly good model of the material, what it does and how it behaves and explaining many properties of those materials. So, this is the basic idea, we have now presuming, we are trying to incorporate the crystal structure information into the model that we have develop.

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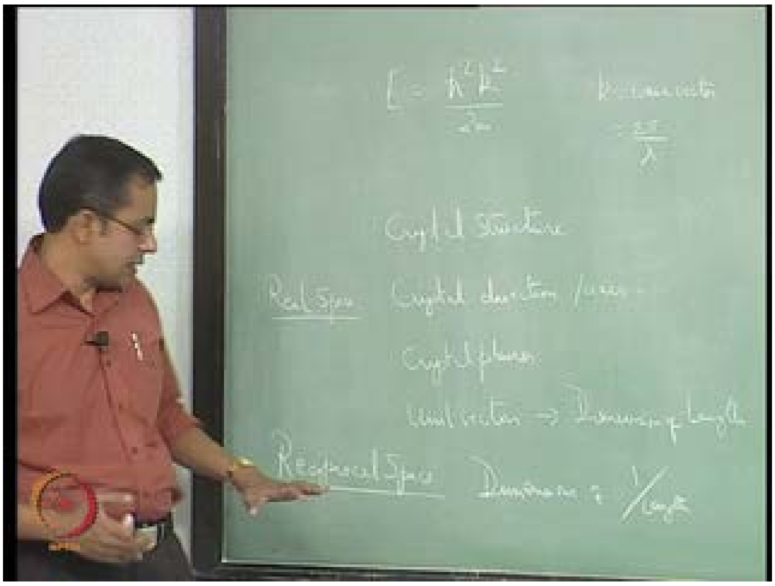

So to do that, we are now going to take a little bit of a d two. So, we we will just start by saying that you know, we have already come up with this relationship between energy and wave vector (no audio from 03:38 to 03:47) where k is the wave vector and is equal to 2 pi by lambda. And in in our context, this lambda here is the wavelength that we are associating the de Broglie wavelength that we are associating those electrons, so that is where this lambda is coming from is not some arbitrary lambda that shows up from somewhere, so it is a lambda that is associated with that particular entity within the material namely the electron. So, we find already, that we are talking in terms of parameter that has the inverse of length as it is dimensions.

So that is something, we will need to keep in mind, what we will, we also recognized that I mean, the crystal structure (no audio from 04:35 to 04:42) is something that you know, in fact you have probably learnt of from high school days and certainly may be early college days, you have heard of crystal structure, you have heard lot of descriptions of it and so on. So, in in those descriptions, you would 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. So these are there, normally these are in dimensions of length.

We basically certainly crystal axis, when we unit vectors we say with respect to so we we define unit vectors dimensions of length (no audio from 05:43 to 05: 51). So, this is how it is done, we write x, y, z coordinate system, we say you know and if you take a real crystal structure you may have specific dimensions in in the in the form of say of the order of say two angstroms inter atomic spacing is of the order of two angstroms, say 1.5 angstroms, 1.8 angstroms, angstroms is ten power minus ten meters, so it is still with the dimensions of length. So, when you normally put such information together, so we would call this as real space (no audio from 06:21 to 06: 27) real space is what we are conventionally use to, which where we write x, y, z coordinate system and within the framework of that x, y, z 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, what we are going to do today is define something that we will call reciprocal space (no audio from 06:54 to 07:03) we will define something called reciprocal space and we will begin to see some of it is properties. Reciprocal space in fact takes the basic approach here is that the same crystal structure information that you have here, are and many of it is important key features can be represented in another format known as reciprocal space. So, we are not actually changing anything in in a fundamental sense, because you are still talking of the same material, you are still talking of the same… I mean same relationship 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 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 (no audio from 07:57 to 08: 07) or length power minus one 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.

So therefore, it it may be, 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, if you use the same 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. So, that is may be a little bit of a trivial way of saying it, but it will it it is it certainly conveys the immediate link between what we have just done up and till now and what we are planning to do.

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 in this reciprocal space actually conveys certain details of how interactions occur between between a crystal structure and waves that are present much more elegantly, then is then is then in real space. So, in a broader sense, this is this conveys certain information much more elegantly reciprocal space and actually is able to highlight specific details 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 mate, 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 the 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. So, it will look like while go to all the you know troubles of creating everything in 1 by length, when real space is already there for us, it is yes that if you use it enough, you find that there is lot of information that is much more elegantly and clearly represented in in when you use this notation then when you use real space notation. So, it is from that perspective that this is really carton.

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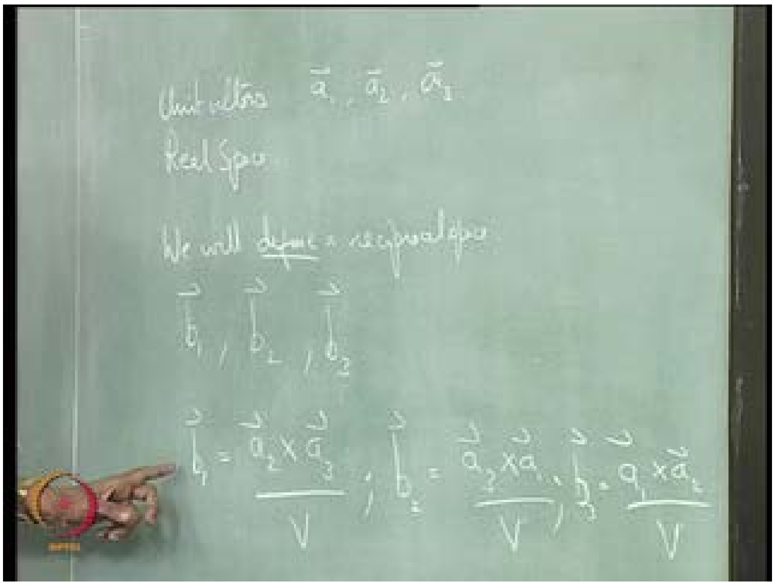

And it traces itself back to a person by name Ewald, who actually worked on this in around the years around the year 1920. So around that time frame was when this work was put together and so there is there is notation, which is which is named after him also in in this relationship. So, in this context, so we will see that as I mention you know we have sort of indicated, why we 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 2 pi by lambda power k wave vector.

And we want to see the interaction between the electron waves and the crystal structure and therefore, it would help if you all if you presented all the information in the same framework. So, we can think of that as a loose link for what, why we are doing what we are did, as we progress forward we will see much more better understanding of how this system works on. So, now we will look at in the next two or three classes, we will actually focus exclusively on reciprocal space and we will build it is relationship to the real 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 for, but we will lead to build this framework, so that we can connect it up link it up to our discussion earlier and see what what benefits we can gain from the process. So, but temporarily for at least this class and 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 real space and also take I mean extend this idea, the diffraction occurs in reciprocal space and it has a certain way of being convey it and see what is the consequence of that discussion, on how the electrons are interacting with the crystal lattice.

So that that step is going to be to at least two classes away, before we get there, but now we will have to build the framework which will enable us to handle that discussion. 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 (no audio from 12:52 to 13: 00) and typically we would use the notation a 1, a 2 and a 3. So a 1, a 2 and a 3 are unit vectors in real space (no audio from 13:14 to 13:20). So, we have a crystal structure in real space represented by these unit vectors a 1, a 2 and a 3.

Now, we will define a reciprocal space (no audio from 13:29 to 13:41) in other words, we will define a space, we will define a coordinate system, so we are just going to define it upfront. 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, so this is a choice we have making, so we are defining it. We are defining reciprocal space to consists of three vectors again unit vectors there b 1, b 2 and b 3, 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 in the process of this definition, we are already making a link between these vectors and these vectors and what is that link, it is it is written like this. So, b 1 is a 2 cross a 3 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 a 1, a 2 and a 3; b 2is defined as a 3 cross a 1 by V and b 3 is similarly is a 1 cross a 2 by V. So, these are cross product, these are vector cross products, so that is what they are, so these are all vector quantities b 1, b 2, b 3 are vector quantities, so they have magnitude as well as a direction a 1, a 2, a 3 are also vector quantities, they all also have magnitude and direction and this is the cross product and so it is defined that b 1 is defined as a 2 cross a 3 by V; b 2 is defined as a 3 cross a 1 by V and b 3 is defined as a 1 cross a 2 by V. 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 b 1, b 2 and b 3, which becomes convenient for our utilization later on.

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 what is the relationship between b b 1 and these reciprocal, so these are called reciprocal lattice vectors, 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 a consequence in in the relationship between b 1, b 2 and b 3 with respect to what we have in real space.

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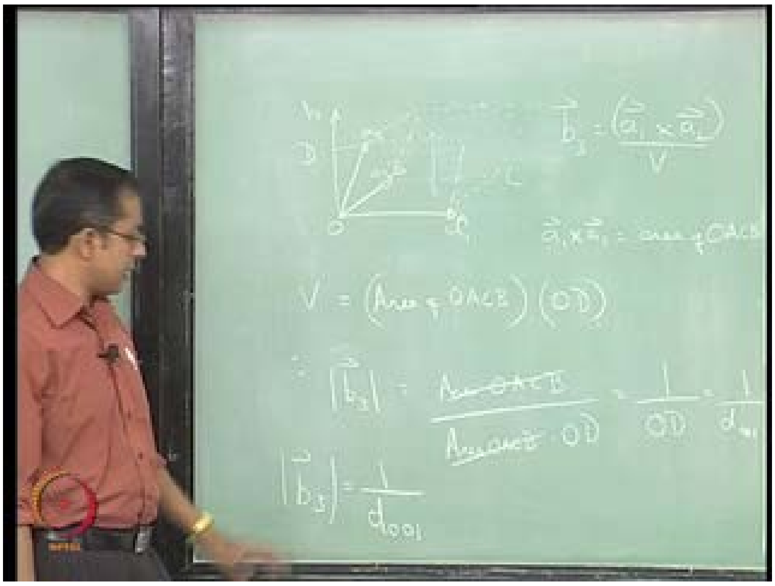

So that is first thing that we will examine, so to do that, let us take an arbitrary say a triclinic cell (no audio from 16:51 to 17:04) a triclinic cell is one, where by definition the a 1, a 2 and a 3 vectors need not have the same length. So a 1 need not be equal to a 2 need not be equal to a 3 and the angles between them. So alpha, beta and gamma, which are the three angles that exists in the system need not be the same, so that is the… So in that sense, it is a it is it is like a very general cell, we have placing, we are really placing no restrictions on it. Now, we are defining we will we will write b 3 again here, (no audio from 17:31 to 17:42) fine a 1 cross a 2 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 a 1 cross a 2 by definition of cross product, if if you have a cross product the the result is perpendicular to both a 1 and a 2, so that is the meaning of a cross product. So, b 3 therefore by definition is perpendicular to a 1 and a 2, so on this scale if you want to draw b 3, it will show up something like this, it will show up somewhere in this direction, it will be perpendicular to the plane being described by a 1 and a 2, so the planes a 1 and I mean the vectors a 1 and a 2 define a plane, which is which we are now treating as the horizontal plane on this board sort of in this representation and b 3 would now appear in this direction perpendicular to a 1 and a 2.

So, that is the definition by way of definition, but what about it is actual magnitude, if you look at a 1 cross a 2, if you if you see the by the standard definition of a 1 cross a 2 that is the area of this parallelogram. So, if you write this as the origin, you write this is O, A let us say this is B and let say this is C. So the area of this parallelogram O A C B, is what is being given by a 1 cross a 2. So, O A C B area of paral a 1 cross a 2 (no audio from 19:11 to 19:23) O A C B 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, so that is the volume, that is that V, so which is that volume, if you take this a 3 vector and you complete this solid (no audio from 19:45 to 19:52) so that solid (no audio from 19:53 to 20:01)

So, this unit cell that we have drawn here, I mean if it 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 in terms of geometrical terms, it simply the area of this base times distance between these planes are the height of this unit cell. So that is all the volume is 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 A, B, C, so this is D lets call this D, O D.

So, O D is the height of this unit cell that we have drawn, and it is simply the projection of a 3 on this on this axis on this axis which is perpendicular to a 1 and a 2 right, so that is the height. So, we will call that, so the height is O D so the height is O D. So therefore, volume is the area of O A C B into the height O D, so it is the product of the area times the height that is the volume. So therefore, if you look at it that way b 3 are the modulus of b 3 (no audio from 21:33 to 21:43) is area O A C B by area O A C B into O D, so that is is what the modulus of b 3 is, so these two will cancel out, so it is simply 1 by O D, so it is simply 1 by O D. So, that is the magnitude of b 3, so b 3 is in this direction and the magnitude of b 3 is simply 1 by O D, what is 1 by O D.

If we look at the conventional planes that we are looking at, if it look at the way, we define planes, this is the 1 0 0 plane. So, if we look at 1 0 0 plane, this is the d 1 1 d 1 0 0 plane it is the spacing between 1 0 0 planes. If you go back to your elementary crystallography, the 1 0 0 planes are defined this way and then these are the 0 0 1planes d 0 0 1 this is perpendicular to a 3 axis. So d 0 0 1, if you want to call it 0 0 1. It is the spacing between 0 0 1planes. So spacing between 0 0 1planes is what we have now look at. So, O D is the spacing between 0 0 1plane, so d 0 0 1, (no audio from 23:01 to 23:08) so b 3 is therefore spacing (no audio from 23:11 to 23:22) this is the standard notation for crystallography, so if you go and look up crystallography from your elementary crystallography, this is the d 0 0 1is the spacing between 0 0 1planes and modulus of b 3 is simply 1 by d 0 0 1.

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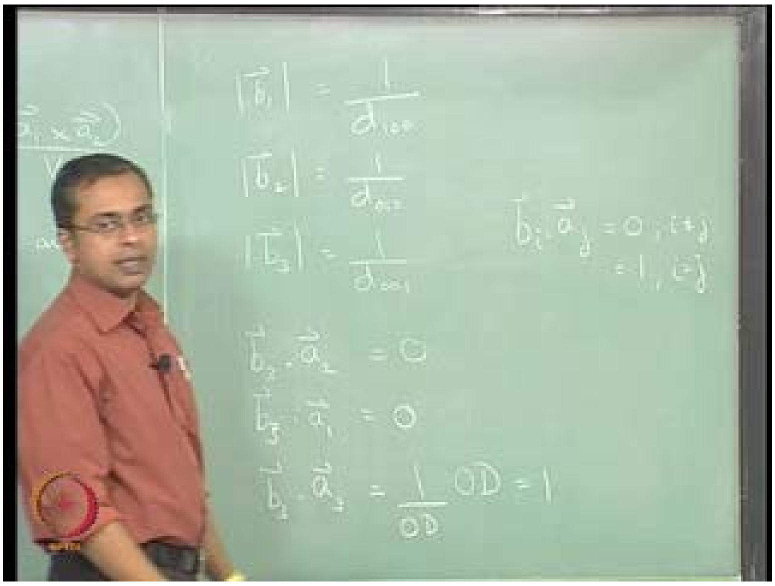

So therefore, we find and by analogy in fact I mean in fact if you extend this argument the same thing would hold for the other ones too, b 1 is 1 by d 1 0 0, b 2 is 1 by d 0 1 0 and b 3 if we just did is 1 by d 0 0 1. So b 1, b 2 and b 3 are inversely proportional to spacing of those planes 1 0 0, 0 1 0 and 0 0 1planes, so that is the… by way of our definition we have created this situation, so it is, so it did not arbitrary occur since we defined this way, this is the way it is occur. Also, if you look at the way we have defined it we will also see that if you just take a product say b 3 cross a 2 or b 3 dot a 2 (no audio from 24:37 to 24:43)

If we just take this dot product between b 3 and a 2, I just arbitrary peak this two vectors. We find that since b 3 is already perpendicular to a 1 and a 2, this dot product is 0, so by definition it will be there will be a cos ninety degrees which shows up here, therefore this is 0, similarly b 3 dot a 3 sorry a 1 equal 0, because b 3 is perpendicular to both a 2 and a 1 simply based on half we have defined it that’s all it is. So therefore, these two are 0, if we look at b 3 dot a 3 based on our definition, if you go back to our the picture we have drawn here b 3 has the is this distance O D, I am sorry this is 1 by distance O D.

So which we just saw here 1 by O D, b 3 is modulus of b 3 is 1 by O D, so this is simply equal to 1 by O D times the projection of a 3 on b 3, 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. So what is the projection of a 3 on b 3 projection of a 3 on b 3 is O D, a 3 on b 3 the projection of a 3 on b 3 is O D as as shown in this diagram fine. So therefore, the dot dot a 3 that we are having in the dot product is simply works out to O D so to speak. So this projection will become O D therefore, this equals to 1, so we fine the relationships between those vectors the the reciprocal lattice vectors and the real lattice vectors based on how we have defined those vectors based on how we have defined those vectors creates the situation, where b 3 dot a 2 is 0, b 3 dot a 1 is 0 and b 3 dot a 3 is 1.

So, more generally if we have b i dot a j then this is equal to 0, when i not equal to j and is equal to 1, when i equal to j. So that is the notation that we have and that is the consequences of what the way which we have define these vectors. Now, we already seen if we have taken a specific case actually where we are saying that if we have the particular vector, so d b 1 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 a 2 and a 3, and it is equal the in magnitude it is equal to 1 by the spacing d 1 0 0.

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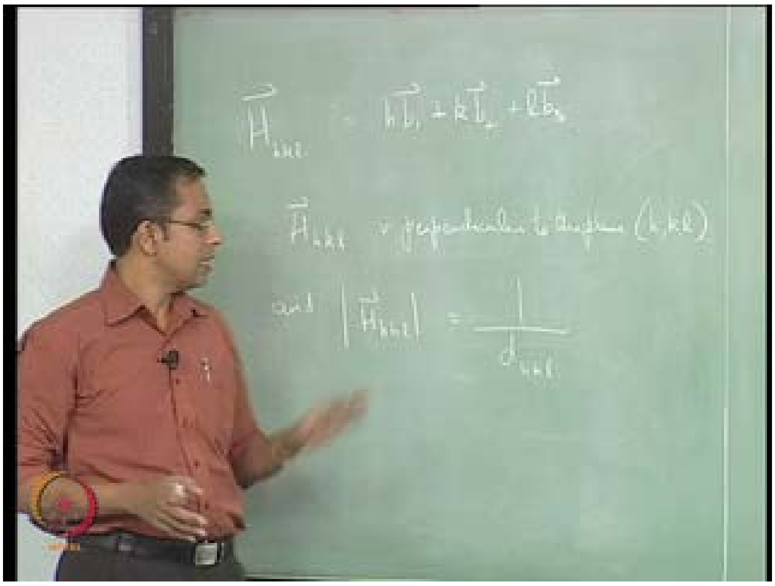

In reciprocal lattice, we can actually generalize this much more, we will generalize it as follows, we can write any vector h h k, H is the notation that is given for a reciprocal, a general, a generic reciprocal lattice vector. So, where we it could be anything, so h is general reciprocal lattice vectors, we will give it subscripts h k l. So, if this is the reciprocal lattice vector and the unit vectors in the reciprocal space are b 1, b 2 and b 3 then this is simply equals to h b 1 plus k b 2 plus l b 3, this is simply based on our definition and and vectorial standard vectorial notation standard vectorial notation b 1, b 2 and b 3 are unit vectors and h k and l are the specific distances we are travelling along those unit vector directions.

So, H h k l is a vector in in reciprocal space and it is therefore equal to h b 1 plus k b 2 plus l b 3 those h k l are the amounts that we are travelling on those respective directions, so that is what it is. We say that, when we define, when unit, when reciprocal space is defined way we have just defined it, then when you take a general vector H h k l in the reciprocal space, we can there are some relationships, it has to real space vectors and dimensions of real space just the way b 1, b 2, b 3 themselves have relationships to the a 1, a 2, and a 3. We just saw relationship between b 1, b 2, b 3 and a 1, a 2 and a 3.

Similarly, we there is a very general relationship between any h k l vectors in reciprocal space and certain quantities in real space, what is that relationship, it is basically that H h k l is perpendicular (no audio from 29:36 to 29: 42) to the plane, which has the miller indices h k l and modulus of H h k l is equal to 1 by d h k l, please note in both these cases we are relating something reciprocal space to something in real space. This is not complicated because we just did that already, when we looked at a 1, a 2, a 3 and b 1, b2, b 3 and we made relationships between them, when I said that no b 1 is 1 by d 1 0 0, b 2 is 1 by d 0 1 0 and b 3 is 1 by d 0 0 1, there b 3 is a reciprocal lattice quantity and d 0 0 1 is a real lattice quantity.

We found that you know simply because of the way we have defined it, in our definition itself we have link real space and reciprocal space, so they are not arbitrary quantities, so they are already link 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 the reciprocal lattice vector and it it is found that it is perpendicular to a plane in the real lattice, which has that similar indices h k and l and the modulus of this reciprocal lattice vector is 1 by d h k l.

These are properties that the reciprocal are in other words 1 by the spacing of h k l planes. So, these are two properties that any vector in the reciprocal space has, as a result of the definition of the reciprocal lattice. So right now, I have just stated it, in in the next few minutes we will prove these two, once we prove these two, we we have a good understanding of what holds in reciprocal space and how it relates to real space and later we can use these two.

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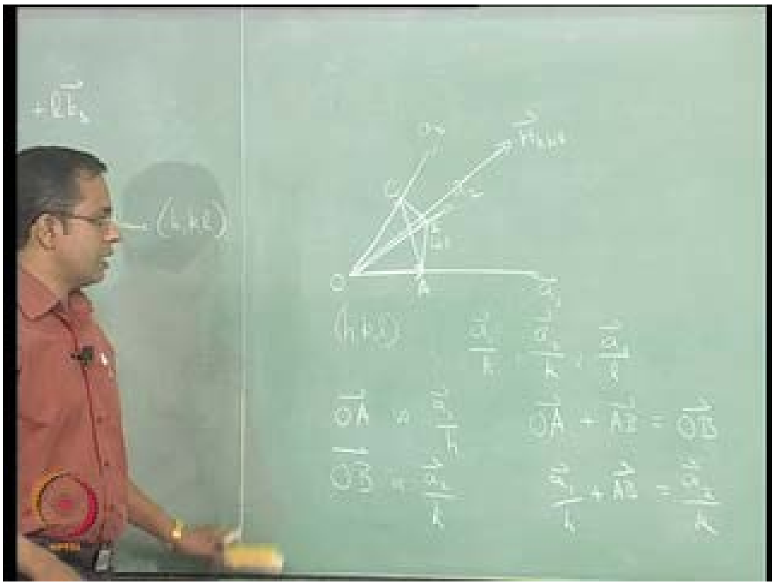

So, we will now try at attempt to prove these, so to do that lets actually draw general plane in the real space. So, we will say that we have, (no audio from 31:49 to 31:57) so this a 1, a 2, a 3, so these are unit vectors in real space and we will draw the h k l plane here (no audio from 32:08 to 31:13) so this is the h k l plane fine. So, now we will just say that in in reciprocal space, we have the H h k l at this moment, I am just arbitrarily denoting it denoting it here, this is an arbitrary denotion at the mom arbitrary denoted it this way, indicated it here in this figure this way. Simply for sake of convenience to show it in the same figure, what relationship it actually has to H h k l it is not forced upon it simply because of how I have drawn it we would 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 h k l plane, it is intercepts along a 1, a 2 and a 3 are simply a 1 by h, a 2 by k and a 3 by l, So these are the intercepts only because the plane h k l happens to intercepts a 1, a 2 and a 3 at those locations, such that it intercepts are at a 1 by h, a 2 by k and a 3 by l, that is the reason why we even fall it the h k l plane. So therefore, if you see, if you take this vector here, this vector here is a 1 by h, this is a 1, a 1 by h is this vector that is why, you will get the h notation in the h k l plane. Similarly, this vector here will be a 2 by k, that is why you get the k notation, this vector here from here to here is a 3 by l, that is why you get that l in the h k l.

So this is a 1 by h, I will also name this locations where this plane intercept a 1, a 2 and a 3 yes A B and C. So, O A is a 1 by h and O B, so this is origin O, O A, O B and O C, so O A is a 1 by h, O B is a 2 by k fine. So, this is what we have, so simply by vectorial notation, if you write O A plus A B you should get O B right. So, O A simply because of standard victorial notation O A, so with this are vectors O A plus A B should equal O B that is easy to see, if we go from here to here and there if we go from here to here it is the same as going from here to here that is all it is, O A plus A B is O B. So, this is what we have (( )). So, now that we know these are the vectors we can replace them O A is a 1 by h and O B is a 2 by k. So therefore, a 1 by h plus A B vector A B should equal a 2 by k fine this is what we have.

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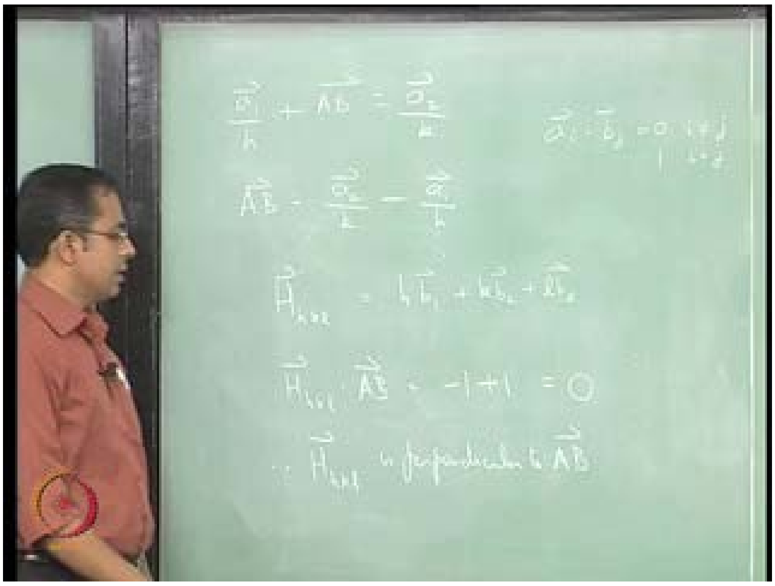

We can rearrange this a little bit, so we wrote a 1 by h plus A B equals a 2 by k, rearranging this we get A B, which is a 2 by k plus sorry minus a 1 by h. So, we now have in terms of the a 1, a 2 vectors we have the vector A B given to us in terms of unit vectors a 1 and a 1 and a 2, which we have already defined for a real space. We already said that if we take vector H h k l we are defining it based on this notation as h b 1 plus k b 2 plus l b 3, so the h k l, h k and l are simply integers, so this is some vector in reciprocal space, so h k and l are just integers. So as long as they just integers, you can use them which ever space you wish they just integers b 1, b 2 and b 3 are reciprocal lattice vectors therefore, h b 1 plus k b 2 plus l b 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 A B it is a real lattice vector, because these are just integers we are which 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 h k l plane is this result in this relationship and the same h k l values we have now used for this definition, although we have got no significant for it they just same enforcing the same h k l in this definition for this H h k l. So if you now take a dot product of H h k l and A B, what will you that, so if you do H h k l dot A B, so we have b 1 here, h b 1 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 equal to 1, if i is equal to j and since it is a dot product, you can have it a i dot b j is the same as b j dot a i, in the order in which you do this dot product is not important to us, because I the way you will get the same that, so if you look at this dot product here, you have h b 1, h b 1 dot a 2, so these are just the h is just an integer b 1 dot a 2 is 0, because one and two here, so that is 0, b 1 dot a 1 is one and you have a h b 1 here and a 1 by h here, so h and h will cancel you get minus 1, h b 1 times or dot product of h b 1 and a 1 by h will give us minus 1.

If we take b 2 here, k b 2 times a 2 by k the k and k will cancel, you have b 2 dot product of b 2 and a 2 which is one plus 1 and this b 2 dot a 1 is going to be 0, because it is subscripts 2, and that the subscript 1 and 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 going to be 0, so this term does not contribute to any way becomes all 0, so this become 0, the product with this gives us a plus 1, the dot product with this gives us a minus 1, so this is equal to 0. So, we have a situation, where vector and reciprocal space H h k l dot vector in real space is equal to 0. So, in other words we have a dot product between two vectors, which is 0, which is simply implies that H h k l is perpendicular to this vector A B.

Therefore, H h k l is perpendicular (no audio from 40:03 to 40:11) so if you go back to our figure, it means that this H h k l is perpendicular to this A B, so this A B is there, the way this H h k l is define, it is perpendicular to A B using exactly the same derivation that we have done, instead of we started with this this location being a 1 by h and this being a 2 by k, we can do the same thing with a 2 by k and a 3 by l. In which case, we will find that H h k l will become perpendicular to B C. Similarly, we can also do it with a 3 by l and a 1 by h and exactly the same calculation, we will do we find that H h k l is perpendicular to A C. So, we find that H h k l is perpendicular to A B, it is perpendicular to B C and it is perpendicular to C A based on the same derivation that we have done.

Simply we have to select the other two axis, you come to the exact same conclusion. The same mathematics will work out in exactly the same way, we will find that H h k l is perpendicular the vector H h k l is perpendicular to vectors A B, B C and C A therefore, and since all of these three are forming a plane, if it is perpendicular to any two in fact even even if it is perpendicular to just two, certainly perpendicular to two and it also perpendicular to all two, if it is perpendicular to then it is therefore, perpendicular to the plane defined by A B and C.

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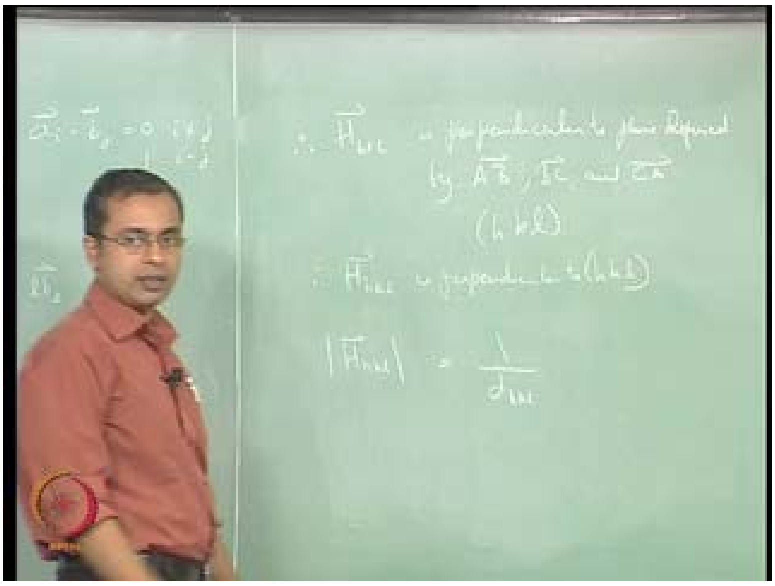

Therefore, H h k l is perpendicular to plane defined by A B C, A B, B C and C A and therefore, which is basically H h, which is basically a h k l plane. So, that is how those vectors are (( )) defined A B and B C and C A were defined based on the intercepts at 1 by h, 1 by k, 1 by l those respective axis. So therefore, H h k l is perpendicular (no audio from 42:25 to 42:31) to h k l. So any, so again we relating something in reciprocal space a vector in reciprocal space to a plane in real space. And again all these relation are coming about simply because are original definitions, related reciprocal lattice vector to real lattice vectors, so that relationship was already there within the framework of this relationship we are re finding other other relationships that hold.

So, we find that any H h k l plane which is therefore, defined as h b 1 plus k b 2 plus l b 3, where b 1, b 2 and b 3 other unit vectors reciprocal lattice reciprocal space, those h h k l vectors will automatically be perpendicular to the H h k l planes in the real space, so this is already we have seen this, so we have just we have just show this. So, the other thing we would like to see is, what is the value of modulus of H h k l and how does this relate to the spacing of between the h k l planes. We will in fact see that this is equal to 1 by d h k l, so this is what we are just about it.

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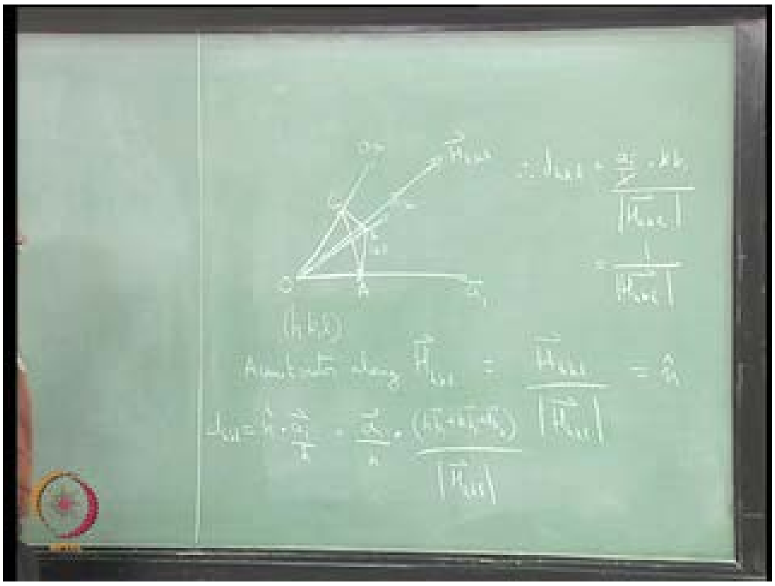

We are going to look at, we will come back to this figure, let us say that a unit vector along H h k l. So, we will let us first define a unit vector along H h k l that is simply H h k l by modulus of h k l of H h k l right that is the definition of unit vector along H h k l. We will just called as the say n, n cap now, when you say h k l plane is defined the way we have just drawn it, when we say this, we mean that the, that there is a similar plane like it at the origin, then there is one at this location, then there is similarly spaced next way similarly spaced next way and so on. That is the way we defined a family of set of planes, when you say a h k l plane it is not just a single plane, I mean it is that is set of planes which are parallel there.

We take the one closest to the origin and then take the intercept of it and that is how we come with h k l, so there are planes corresponding so therefore, the spacing between the h k l planes is simply the distance between the origin and this h k l plane right. The closest distance or other 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 d h k l. So now, we have basically seen that the at at that point the he line drawing from the origin, which goes closest to this plane will then go perpendicular to that plane.

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 H h k l or n cap dot a 1 by h. If you take the dot product of a 1 by h and you take it is, what should I say the the the dot product of O A with this vector in the direction of this H h k l then you get the component of O A along the direction and that would then be the spacing that you are interested. So this is what you will get, so this is simply a 1 by h dot product with you will have h b 1 plus k b 2 plus l b 3 divided by the modulus of H h k k. So, this is d h k l right.

So, d h k l is now defined this way d between those planes is such that the if you take the the component of any of those intercept along the perpendicular to that plane. So, that perpendicular is now going through that origin, so that perpendicular vector that is there, if you take the component of this vector along the direction of that perpendicular you therefore, get the distance in this direction. So that vector, unit vector is simply giving as the direction there, but if you take the component of this intercept O A along the direction or any of those O B along the direction or O C along the direction.

If we 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 and that point that vector will be perpendicular to that plane, which is what how we have defined. So, if we 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, the d spacing of that plane, because the next plane is sitting at the origin. So, d h k l is the component of this vector a 1 by h along this unit vector here, the unit vector is simply defined by this and this and since it is a dot product we can interchange the it 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 a a 1 here, we have a b 1, b 2, b 3 here, and clearly a 1 dot b 2 is 0 and a 1 dot b 3 is 0 the way we have already see. So, only a 1 dot b 1 is going to count for anything else, so a 1 dot b 1 is going to be, because of the way it is defined and the h and h was are going to cancel therefore, d h k l is equal to a 1, so we just write it here, a 1 by h dot h b 1, b 1 or a 1 a 1 dot h by h b 1 dot h b 1 divided by modulus of H h k l, so this and this will cancel a 1 dot b 1 equals one, therefore this is equals to 1 by H h k l.

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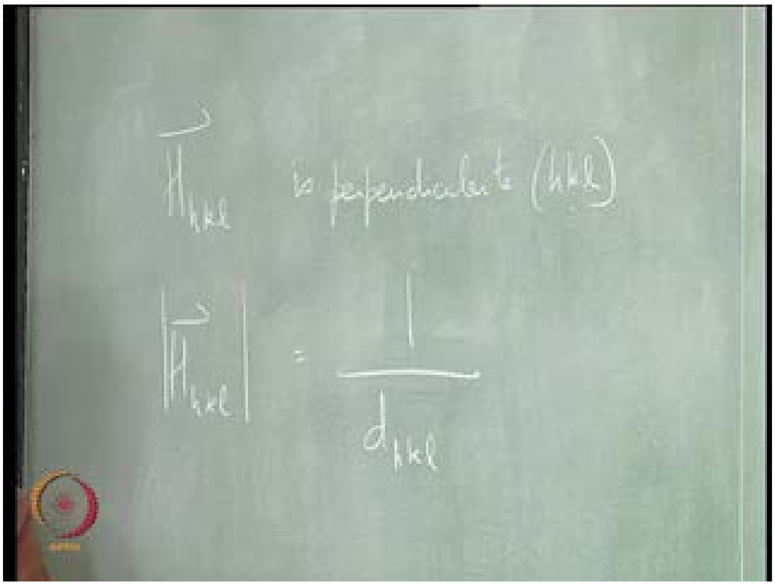

So we see, which is the proof that we wanted to we set out to prove, so we see that H h k l is perpendicular to (no audio from 49:36 to 49:45) and modulus of H h k l equal to 1 by d h k l. So, what we have seen is, we started of this class by saying that we need notation which is this reciprocal lattice notation, because it will helps us understand the interaction between the wave vectors corresponding to the electrons, and the crystal structure, which is which basically conveys to us the periodic structure that is presents 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 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 defined reciprocal lattice to be consisting of b 1, b 2 and b 3 with specific relationships to the real lattice vectors a 1, a 2 and a 3, on the strength of that relationship, we found that on the strength of the definition, we found that already b 1, b 2 and b 3 had specific relation to a 1, a 2 and a 3, which then translated to a general reciprocal lattice vector H h k l having specific relationships to the plane h k l in real space. The relationship are at the vector H h k l is perpendicular to the plane h k l 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 h k l planes. 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 phenomenon can be represented in the reciprocal lattice notation. When we understand that, we will then be able to take it forward and see what happens when you have electron waves travelling through a crystal structure, which has a periodic structure associated with it. And therefore, we will see how all of this material that we are currently discussing will enable us to have better insides with how the material function and how it is properties evolved, because of the structure there present within the material, and the facts that this electrons are travelling through that structure with the wave like phenomena behavior. So, with that we will hold for this class, we will pick it up in the next class with some more discussion on reciprocal space, before we take it is utility and extract more information, thank you.