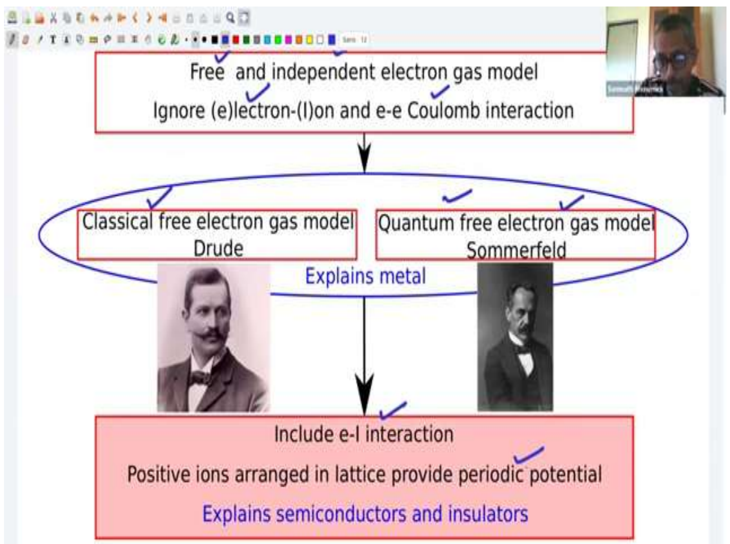
Electronic Properties of the Materials: Computational Approach
Prof. Somnath Bhowmick
Department of Materials Science and Engineering
Indian Institute of Technology – Kanpur

Lecture – 16
Real Lattice and Reciprocal Lattice

Hello friends, in this lecture we are going to discuss about Real Lattice and Reciprocal Lattice.

(Refer Slide Time: 00:21)

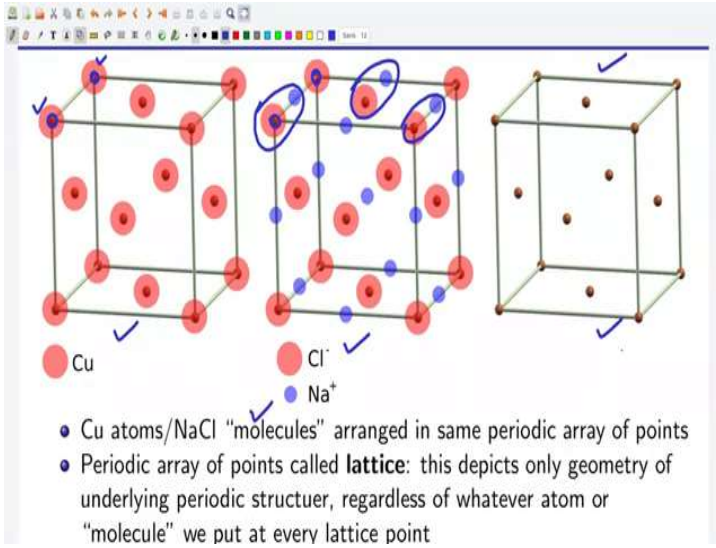


Let us first briefly discuss, why do we need the concept of lattice? So, we started our discussion with free and independent electron gas model and we ignore electron ion and electron-electron coulomb interaction. First, we discuss the classical free electron gas model and then we discussed quantum free electron gas model. We have found that certain anomalies observed in classical free electron gas model like the magnitude of the heat capacity was resolved, by using the quantum free electron gas model.

However, certain other anomalies like sign of the all coefficient could not be resolved even after using the quantum free electron gas model. Thus, we concluded that the sign anomaly of all coefficient cannot be understood using free electron gas model at all. Thus, we need to include the electron ion interaction.

And positive ions arranged in lattice provides a periodic potential and we need to solve the Schrodinger equation in the periodic potential. So, before we do that let us briefly understand the concept of lattice in this lecture.

(Refer Slide Time: 01:43)

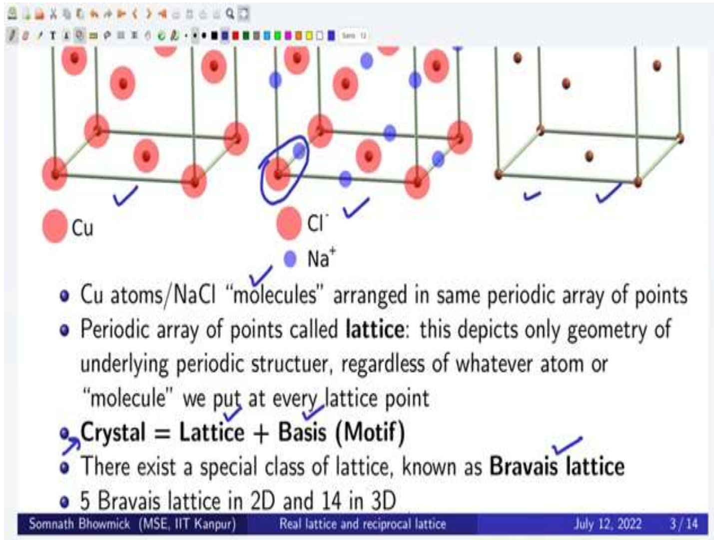


Picture of copper and sodium chloride crystal is shown here side by side. This is how the copper atoms are arranged in a copper crystal and this is how sodium and chlorine ions are arrange sodium chloride crystal. Do you find any similarity between the two? Now, let us focus on this small small points, right. In case of copper crystal, what we do is that we place a copper atom in place of all these small points.

But in case of sodium chloride what we are doing is that we are placing a sodium chloride molecule in place of all these small points. So, you can see that in place of every small point we are putting this sodium chloride molecule. Note that these are not really molecules but these are like just the sodium and chlorine ion pair. Now, instead of the actual atoms are ions if we consider that only the imaginary points then, what you get is a lattice.

And this shows the underlying periodicity of the crystal. Thus, you see that this copper and sodium chloride both of them have same underlying periodicity, and this is shown by the lattice points.

(Refer Slide Time: 03:20)

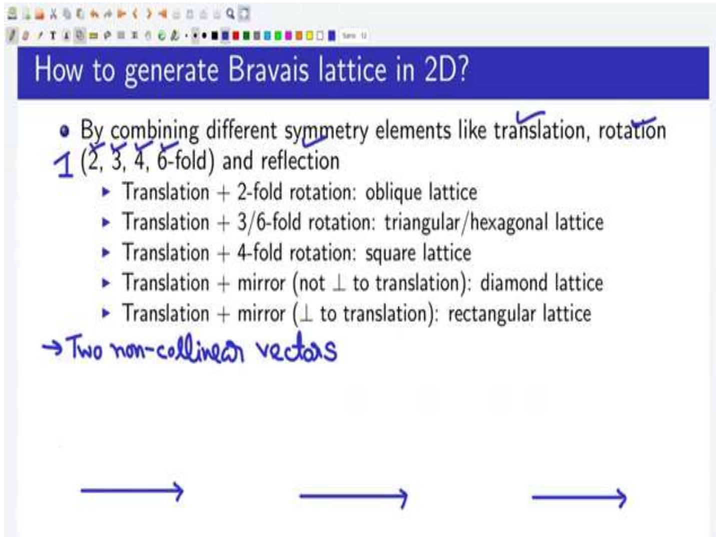


The periodic array of points this is called the lattice, right. This is what is shown here right and this depicts only the geometry of the underlying periodic structure, regardless of whatever atom or molecule we put at every lattice point. We can say that a crystal it is made of two things lattice and basis so, we have this imaginary lattice points and what is the basis in case of copper? The basis is just a single copper atom.

So that means that each imaginary lattice point we put a copper atom and that will give me the copper crystal. And in case of if we want to build the sodium chloride crystal, what we have to do is that? In place of every lattice point we have to put a sodium and chlorine ion here, like this and that will build up. So that is the basis, right, in case of sodium chloride, the basis is a pair of ions,right, sodium and chlorine, okay so that is how to get a crystal.

Now, there exists a special class of lattice and those are known as like the base lattice. There are five Bravais lattice in 2D and 14 in 3D. Let us briefly discuss about them

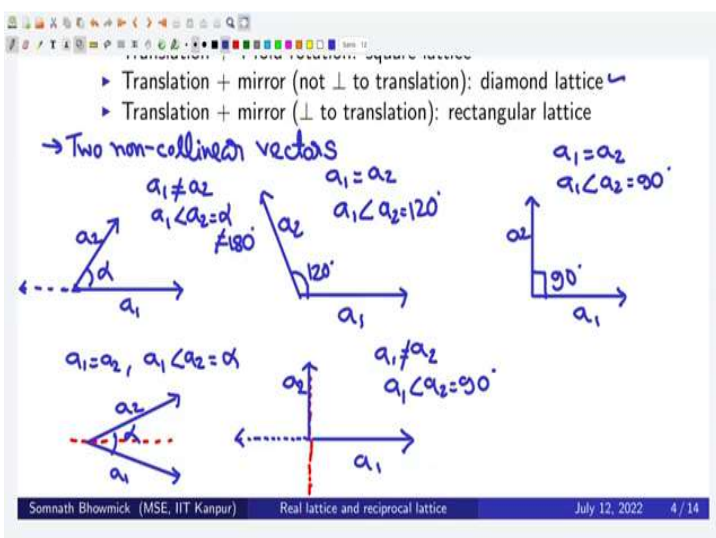
(Refer Slide Time: 04:41)



A 2D crystal has three types of symmetries translation, rotation and reflection. Only five types of rotations are possible if we want to preserve translation symmetry and those are like 2-fold, 2-fold is 180 degree rotation, 3-fold 120 degree rotation, 4-fold 90 degree rotation, and 6-fold that is 60 degree rotation. I did not list out, the other possibility is like 1-fold that is a 360 degree rotation which does not give you anything new.

We shall generate all possible 2D Bravais lattice by combining translation with rotation and reflection. Before we start note that we need two non-collinear vectors to define a 2D lattice.

(Refer Slide Time: 05:38)



So, let us take this case right. So, we take the first vector right to be a 1 and what we need? We need another vector to define a 2D lattice. So, first combine translation with 2-fold rotation, right. So, in this case if we apply 2-fold rotation then what we get is, we get this vector, right, we get some vector which is in this direction right because I have rotated it by 180 degree, right. But this does not give me another non-collinear vector.

So, we are getting the same vector but in the opposite direction. So, what we need to do is that, we can just put the other vector right in a manner that such that it is non-collinear so, we can just take this, right. So, let us put a 2 here correct and then what we see here, right. So, in this case there is no restriction on the second vector, right. So that means a 1 is not equal to a 2 and they have some angle and then the angle is also there is no restriction, only the thing is that it cannot be 180 degree.

Because the 180 degree will give you the same vector that will not give me two non-collinear vectors. So, a 1 angle a 2 is equal to some general angle alpha which is which cannot be equal to 180 degree, right, so, this is the angle alpha. Next, we take a vector again a 1 and then what we do is that? We combine it with 3-fold rotation, right. So, 3-fold rotation is like the uh 120 degree rotation, right. So I get the second vector in this direction.

So that means the rotation by 120 degree. So, this angle is now fixed 120 degree. That already gives me another vector which is non-collinear and in this case how these vectors are related. So now, a 1 the magnitude of a 1 is equals to magnitude of a 2 and the angle between them is. That is also fixed that is equal to 120 degree. Now, I just leave it as an exercise for you to verify that if we try to combine the translation with 6-fold rotation, we get the same lattice.

So, next what we do is that, we take this lattice vector a 1 and then what we apply is we apply the 4-fold rotation. right. So, in that case the second vector is along this side so, this is a 2 and this angle is 90 degree. So that means again we see that we already have just by the rotation, we already have another vector which is non- collinear here, right. So, in this case the lattice vectors they are related by a 1, magnitude of a 1 is equals to magnitude of a 2 and the angle is given by 90 degree.

So now, we have exhausted all possible combinations of translation and rotation. Now, let us combine translation and mirror. So, again we take the the first vector along this direction and then what we do is that, we put a mirror plane. So, we put a mirror plane which is not perpendicular to this vector, okay. So now, if we do that then what happens is that because of this mirror plane right I get so, this vector gets reflected correct then that means I get another vector which is here.

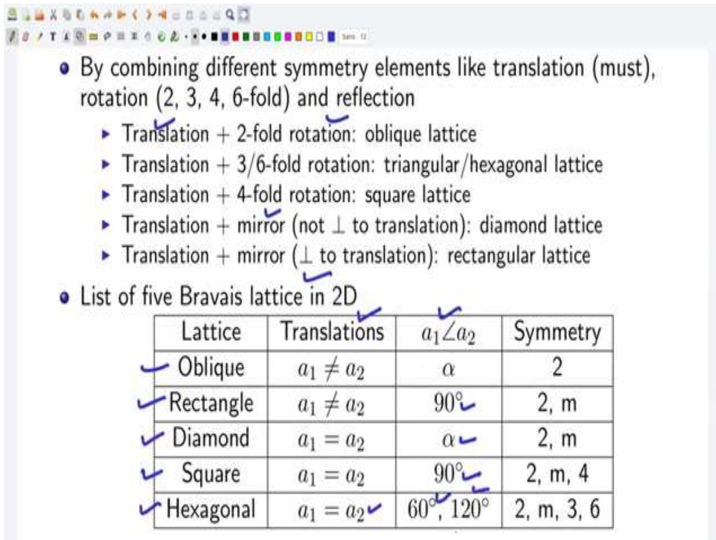
And that already gives me the second vector which is like non-collinear. So, in this case how these translation vectors are related? So, they are related by the magnitude of a 1 is equals to magnitude of a 2. And the angle between them can be in general angle, a 1 angle, a 2 this is equal to some general angle alpha, right. So, this will just call it as alpha, okay. So, we are done with this now, we can put the mirror in some other way.

For example, what we do is, we can put the mirror perpendicular to the first vector, correct. So, let us put the mirror in this direction which is perpendicular to the lattice vector a 1. And then we see that it will do it in that way then I get another vector, correct but this is not non collinear. So that means this will not give me another vector which is non-collinear and then we have to put the the second vector in some direction.

So and then I just leave it as an exercise for you to prove that the only direction in which we can put the other vector is along the mirror. If we try to put any other direction that will give me a third vector and then there is some redundancy and that and then things are not well defined correct so, you cannot do that. The only place we can put the second vector is along the mirror.

And then that gives me this relation, correct, a 1 is not equal to a 2 right and then angle between them a 1 angle a 2 that is fixed that is equal to 90 degree.

(Refer Slide Time: 11:42)



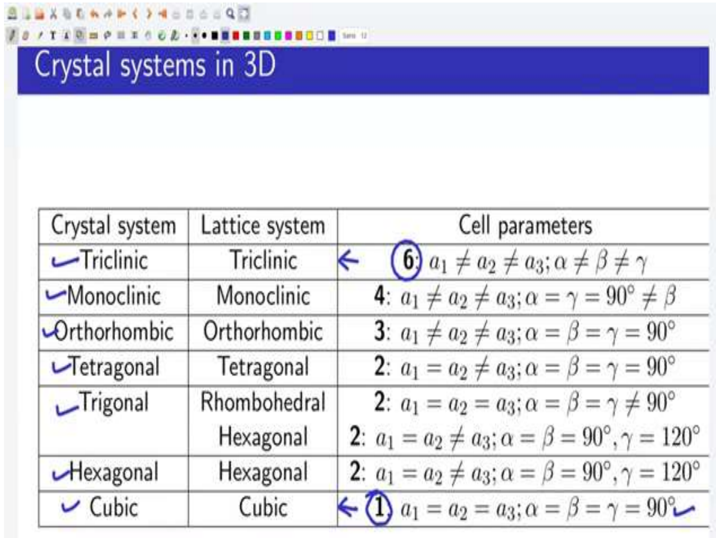
Lattice	Translations	$a_1 \angle a_2$	Symmetry
Oblique	$a_1 \neq a_2$	α	2
Rectangle	$a_1 \neq a_2$	90°	2, m
Diamond	$a_1 = a_2$	α	2, m
Square	$a_1 = a_2$	90°	2, m, 4
Hexagonal	$a_1 = a_2$	$60^\circ, 120^\circ$	2, m, 3, 6

Thus, we have generated all possible Bravais lattice in 2D by combining translation with rotation and combining translation with reflection symmetry. Now, this is the complete list and we also have derived the relation between the two lattice translation vectors, their magnitudes as well as the angle. So, the first one where this has the least symmetry, right so, this is like the the magnitudes are different of the two vectors.

And the angle between them is also some general angle alpha so, this is known as the oblique lattice, the second one is known as the rectangular and in this case the magnitudes are different but the angle is fixed. The third one is diamond, where you have the magnitudes of the two vectors are equal but the angle is general. The fourth one is square, where the magnitudes of the two vectors magnitude is equal and the angle is also fixed equal to 90 degree.

And then hexagonal lattice is again the magnitude are equal and the angle can be either 60 degree or 120 degree, and they are same.

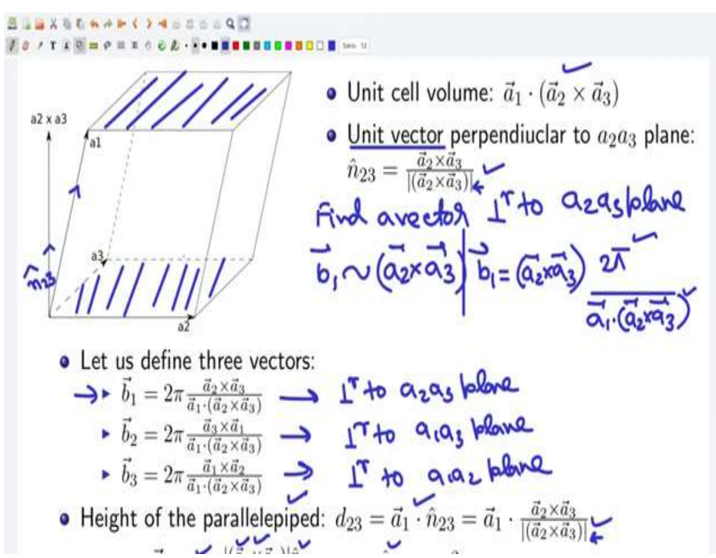
(Refer Slide Time: 13:02)



In case of 3D, we are not going to derive the lattices but using the same principle we can derive them. There is a list of seven possible crystal systems in 3D and you see that the names are like triclinic, monoclinic, orthorhombic, tetragonal, trigonal, hexagonal and cubic. So, in case of this triclinic, this has the least symmetry and then you see that we need like six cell parameters to describe them.

The magnitudes of all the lattice translation vectors now there are like three of them. So, their magnitudes are different and the angles are also general. And then as we go down then we see that the cubic has the highest symmetry and we need only one that is parameter in this case. And that is just because lengths of all the lattice transition vectors are equal and the angle is also fixed and equal to 90 degree.

(Refer Slide Time: 14:02)



We already have discussed about lattice in 2D and 3D. Let us now discuss about reciprocal lattice. We keep our discussion very general by choosing a triclinic unit cell having least symmetry among all. First note that, so, this is the cell right so, we have like a 1, a 2 and a 3 these are the three lattice translation vectors. So, their lengths are not equal and angles are also general. The volume of the unit cell is given by a 1 dot a 2 cross a 3, right.

So, a 2 cross a 3 is the area of this base and then if you just take a dot product with a 1 that will give you the volume of the unit cell. Now, find a vector perpendicular to a 2, a 3 plane, right so, this is the plane, the plane at the base. And then what we can do is that, we know that if we take a cross product of these two vectors right a 2 and a 3 that will be perpendicular to this a 2, a 3 plane.

So, let us do that. So, we know that the vector is given by a 2 cross a 3, right. So, this is the vector perpendicular to this length so, b 1 it is like a 2 cross a 3. So, we take this vector, we multiply it with 2 pi and divide it with the volume, ok, a 1 dot a 2 cross a 3. So, this is the definition of b 1, right. So, b 1 is a vector uh which is perpendicular to this a 2, a 3 plane. And then we have like multiplied it with some constant.

And then with the volume and then you will see that what will be the magnitude of the vector. At the moment, we just know the direction of this vector, right. So, this direction is perpendicular to a 2, a 3 plane. Then we have another vector b 2 which is perpendicular to a 1, a 3 plane and then we have another vector b 3 which is perpendicular to a 1, a 2 plane. Now, let us convince ourselves that the b vectors have a dimension of one over length and it is magnitude is inverse of inter planar distance.

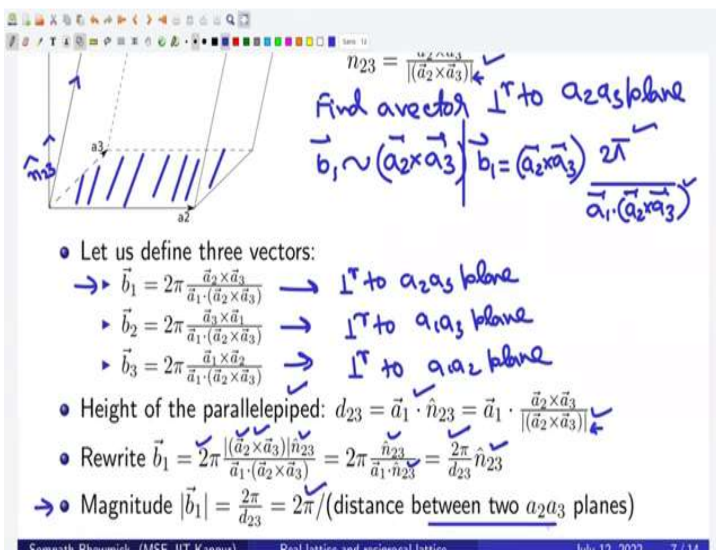
So, let us take d 1 right and then we see that this height of the parallelepiped right this length d 23. right That is given by a 1 dot n hat 23, where n hat is a vector, this is the unit vector correct, n hat is the unit better perpendicular to the a 2, a 3 plane. So, what we do is that, we just take the vector which is perpendicular to a 2, a 3 plane and divide it with it is magnitude, so that will give me the unit vector, right.

And then we see that the height of the parallelepiped that is given by a 1 dot n hat 23, right. And then we just place in case n hat 23 just place this a 2 cross a 3 and divide with it is magnitude. We rewrite b 1, ok so, b 1 equal to 2 pi and a 2 cross a 3 is a vector right so, we just take it as magnitude and then uh n hat 23 is it is direction and then of course this is divided by the volume so, n hat 23 it is already there.

And then if I just divide a 2 cross a 3 by it is magnitude right then I get this n hat 23, right. If I take a dot product of a 1 and the unit vector in this direction right so that will give me the projection of a 1 along this n hat 23 right and that is equal to the height or that is equal to the spacing between these planes. right, so for example, right we can take this to be there to a 3 plane and then we can take another plane which is parallel to this, correct.

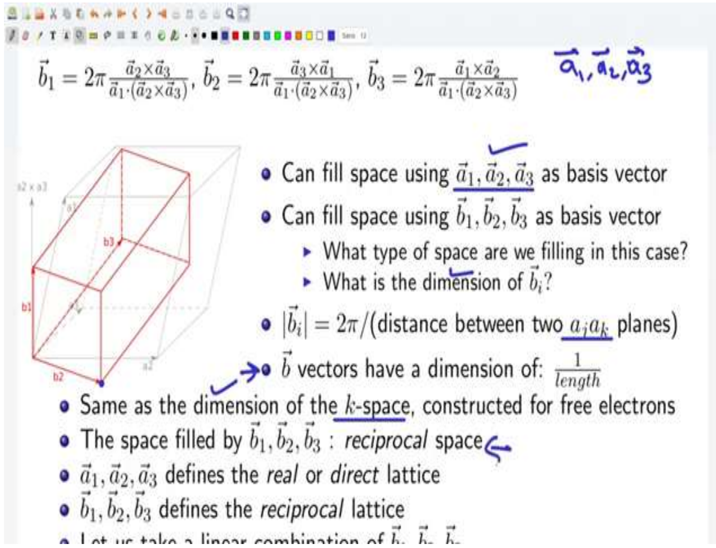
So, if we take this set of planes right then what we can define is that, what is the distance between distance means the perpendicular distance between these set of parallel planes and that will be given by d 2 3.

(Refer Slide Time: 19:11)



So, we can write d 1 as this right so, this is like 2 pi divided by d 23 which is the inter planar spacing between two adjacent parallel a 2 a 3 planes times the unit vector, right along in this direction. So that means we already know the direction of the b 1 so now, thus we have like found the magnitude of b 1 so, magnitude of b 1 is given by 2 pi divided by d 23 that is 2 pi divided by distance between two a 2, a 3 planes.

(Refer Slide Time: 19:43)

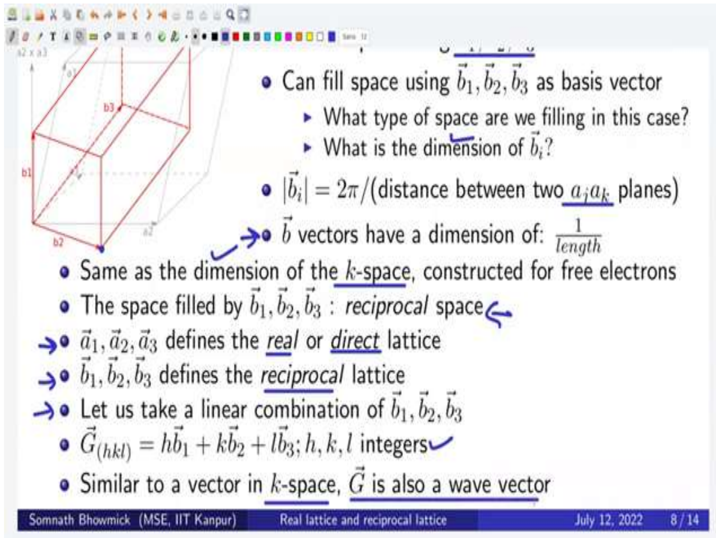


Thus, starting from the lattice vectors a 1, a 2 and a 3 we have constructed three vectors b 1, b 2 and b 3. Now, we can fill space using a 1, a 2, a 3 as basis vectors, correct. So that means if we take this a 1, a 2, a 3 and we just keep repeating them in space then we are going to fill the entire space. In this case it is not too difficult to understand the space filing as all these vectors like a 1, a 2, a 3 this has the dimension of length.

Now, you see I have also drawn the b 1, b 2 and b 3 vectors. So and again you see that if I just repeat these vectors right then we are going to again fill the space. But now in this case, what type of space are we filling? To understand this let us focus at the dimension of b vectors. okay. So, we know that this uh magnitude of b i equal to 2 pi divided by distance between two a j, a k planes and this implies that the b vectors they have a dimension of 1 by length.

Remember that when we discussed about the k-space in case of free electrons, right, the vectors in k-space also have the same dimension that is the dimension of 1 by length. So, since b vectors have a dimension of inverse length space fill by b vectors is known as a reciprocal space.

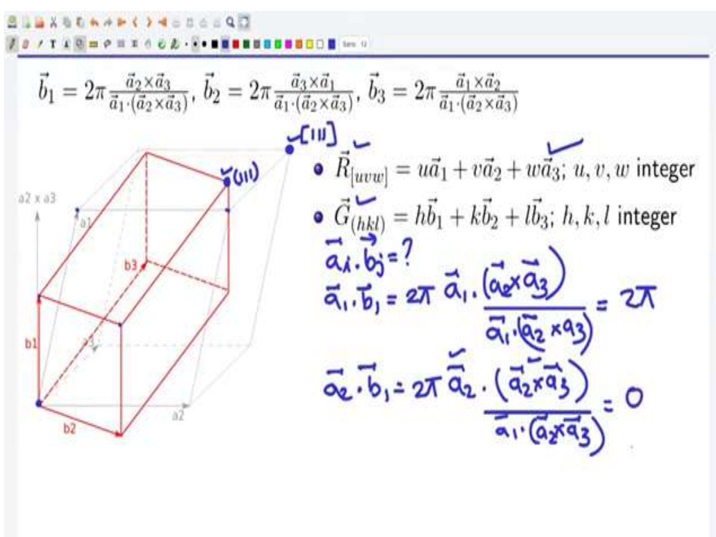
(Refer Slide Time: 21:35)



We call this the lattice spawned by a 1, a 2 and a 3 as the real or direct lattice and that is formed by the b 1, b 2, b 3 this is known as the reciprocal lattice. Now, we can just take a linear combination of b 1, b 2 and b 3 that will give us a vector in the reciprocal space. For example, if we take a combination of a 1, a 2, a 3 right that will give us a vector in the real space. Similarly, if we take a linear combination of b 1, b 2, b 3 that will give us a vector in the reciprocal space.

We know that wave vectors in case k-space, they have a dimension of 1 over length and now, G has also the same dimension of 1 over length so that is why we can argue that this G is also a wave vector.

(Refer Slide Time: 22:40)



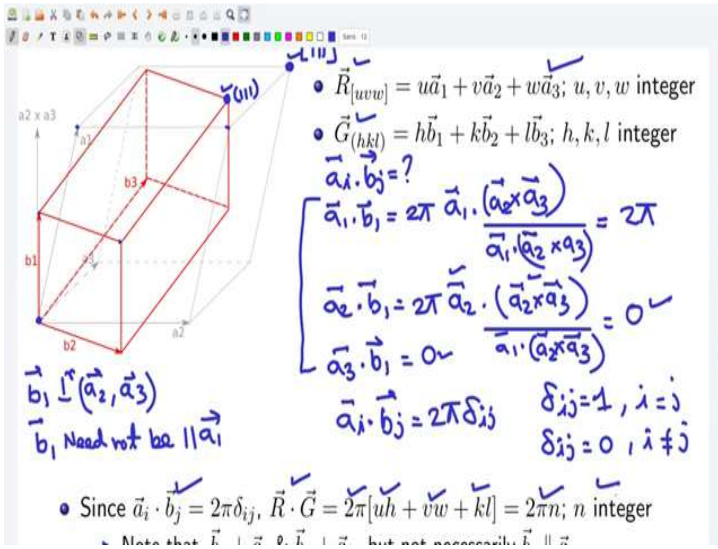
So far we have defined the basis vectors of real lattice given by a 1, a 2, a 3 and the basis vectors of the reciprocal lattice given by b 1, b 2 and b 3. Now, a general vector in real space they can be expressed in this form, R uvw is equals to u times a 1 plus v a 2 plus w a 3. For example you can take this point correct and then you see that how do I reach this point starting from the origin, right, so that means, this is the origin.

So, I move along a 1 by 1 unit, I move along a 2 by 1 unit and I move along a 3 by 1 unit, right. So that means this is the 1, 1, 1 point in real lattice. Similarly, we can write a general reciprocal lattice vector as G hkl, this is equal to h times b 1 plus k times b 2 plus l times b 3 where h,k,l are integers. Again, so for example let us take this point in the reciprocal lattice so, what we do is that, we move along b 1 by 1 unit, we move along b 2 by 1 unit.

And we move along b 3 by 1 unit and then this is the 1, 1, 1 point in the reciprocal lattice. Now, can we take a dot product between R and G? We have to know how does a i dot b j look like. right, okay. So, let us take some examples so, let us try to calculate a 1 dot b 1 so, a 1 dot b 1. So, we are trying to find this and then let us calculate this okay so, a 1 dot b 1 is 2 pi and a 1 is this and what is b 1? b 1 is dot a 2 cross a 3 and then I divide by a 1 dot a 2 cross a 3 correct.

And then what you see is that, we have the same term in the numerator as well as the denominator. So, this we just write it as right so, this this will cancel out right and then we just get a term of 2 pi. Now, let us calculate a 2 dot b 1, in this case what we see is that, we have this factor of 2 pi and then we have a 2 dot a 2 cross a 3 divided by a 1 dot a 2 cross a 3. Now, you see that a 2 cross a 3 is a vector since this is the cross product, this is a vector which is perpendicular to both a 2 and a 3.

So, in that case I am taking a dot product between two vectors which are perpendicular to each other and so that means this term will be 0, correct. So that means a 2 dot b 1 is equals to 0.
(Refer Slide Time: 26:05)



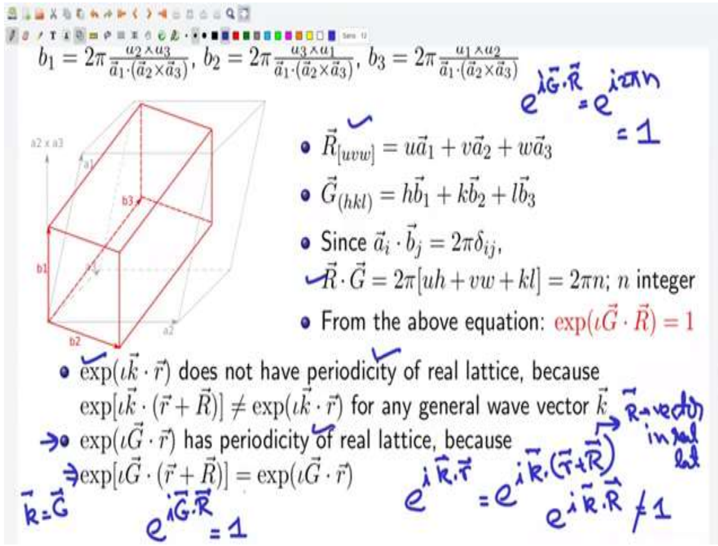
By the same logic we can just show that a 3 dot b 1 will also be equal to 0, right. Remember that what we know is that so, by the the way we have constructed b 1, b 2 and b 3, what we have is that, we know that b 1 is perpendicular to a 2 and a 3, correct. Because we know that b 1 is a vector which is perpendicular to this a 2, a 3 plane and this vector a 2 and a 3 they are lying in this plane.

So that means b 1 is perpendicular to both a 2 and a 3 and that is why this is not surprising that the dot product is 0. But it is not necessarily true that b 1 right so that is b 1 need not be parallel to a 1. They can be in some special cases but if we take a general case they need not be parallel. Thus, these three equations right we can write in a nice compact form in this way, okay. So, a i dot b j equal to 2 pi delta ij.

So, delta ij is the dirac delta so that means delta ij equal to to 1, when i equal to j and delta ij equal to 0, when i is not equal to j. Now, we can just use this fact and then we can take a dot product between R and G. So, R dot G will now look like uh a 1 dot b 1 correct and a 1 dot b 1 equal to to 2 pi correct. And now, you have all these other terms right a 1 dot b 2 that will be equal to 0, a 1 dot b 3 will be equal to 0 and so on.

So that means only the terms like a 1 dot b 1, a 2 dot b 2 and a 3 dot b 3 will be non-zero. Rest of the terms will be equal to 0 and they are given by uh plus vw plus kl and since you like uvw and hkl all of them are integers. We can just we get something like 2 pi n where n is an integer. So, this is how the dot product between R and G right R is a vector in the real space and G is a vector in the reciprocal space. So, this is how their dot product looks like.

(Refer Slide Time: 28:45)



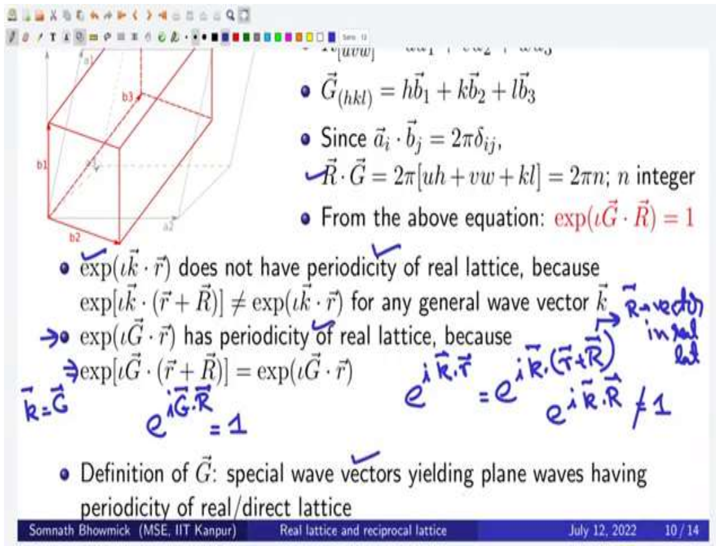
Since, R dot G equal to 2 pi n, we can just take exponential right we can just write it as e power i G dot R equal to e power i 2 pi n equal to 1. Now, let us take some plane wave e power i k dot r, right so, let us take this expression and let us examine whether this has the periodicity of the real lattice. Let us see that what do we need for it to have the periodicity of the real lattice? right. So, what we need is that e power i okay k dot r right for it to have the periodicity of the real lattice.

What we need is that e power i k dot r plus R, where R is a vector in the real lattice. R vector in real lattice, and then you know that R as this form, okay. And now what we need for these two things to be equal, what we need is that e power i k dot R has to be equal to 1. But we know that for some general wave vector k this is not true, okay this is not true for some general wave vector. So, thus if we take some plane wave which has this form we call i k dot R then that does not have the periodicity of the real lattice.

However now, if I take the wave vector to be capital G then let us see that what happens? right. So, we have also defined like some, we know that G is some wave vector, right. So that means if we just take k equal to G right the wave vector we take to k equal to G, in that case what do we have? In that case, we need to satisfy this equation, okay, and then we see that this equation is satisfied because we know that e power i G dot R.

We just have derived it here, e power i G dot R equal to 1. So that means if we take the plane wave with wave vector equal to G then in that case such plane waves have the periodicity of the real lattice.

(Refer Slide Time: 31:34)



Thus, so, G these are like special wave vectors which will give us some plane waves having the periodicity of the real or direct lattice.