Crystals, Symmetry and Tensors
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Lecture 2a
Unit Cell, Basis, Fractional Coordinates

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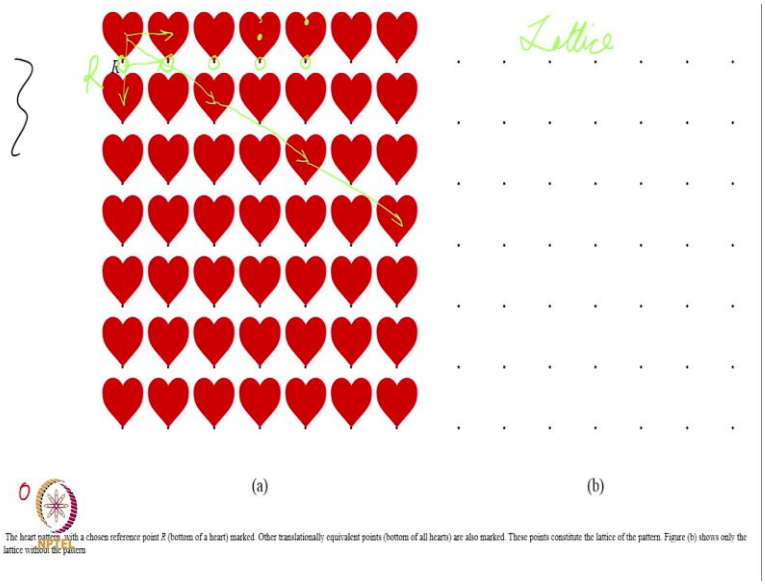

The heart pattern with a chosen reference point R (bottom of a heart) marked. Other translationally equivalent points (bottom of all hearts) are also marked. These points constitute the lattice of the pattern. Figure (b) shows only the lattice without the pattern

So, here we see a heart pattern. And this is a periodically repeating pattern. So, hearts are repeating in two directions, horizontally and vertical. And of course, as you know that any linear combination of these two vectors, if you select, it will be repeating in that direction also. So, if I see a heart at this vector in that direction, if I continue my journey, I will keep seeing identical heart in that direction.

And not only that, I have to get a heart at the right location, I also have to get the heart in the correct orientation. So, suppose if I tilt the heart or turn it upside down, or by 90 degree at the same location, matching the centroid, but rotating the heart then the periodicity is lost. So, not only the positions should be repeated at that position, the same objects should come and that same object should come in the same orientation.

So that is what is being seen in this heart pattern also all hearts are identically oriented. Now, if we select, so, we want to derive the lattice, this is a pattern there is not a lattice, but a lattice belongs to this pattern. And to extract the lattice out of this pattern, I select a reference point which I have called this R here, the reference point which is the bottom of my heart. So, from the bottom of my heart, I go to another heart and there also I select the bottom.

So, identical feature of all the hearts has to be selected not that if I select the bottom here and then if I select the centroid here, and then I select this depression, their depression of hearts is also very common these days. You may like select that, but then you have to keep selecting the same identical points in all, all the hearts. So here I am selecting bottom point, and if I select all the bottom points, then the lattice I get is here.

So, I get a lattice. So, I removed the heart now, because I want to focus exactly on what is the repeat structure or what is the pattern which is repeating. So, that gives me this square grid of lattice points. So, I know that with each lattice point, a heart is associated, or something is associated. If you do not tell me heart, then also, I will know that I am talking about some repeating pattern, where whatever is repeating has this repeat structure.

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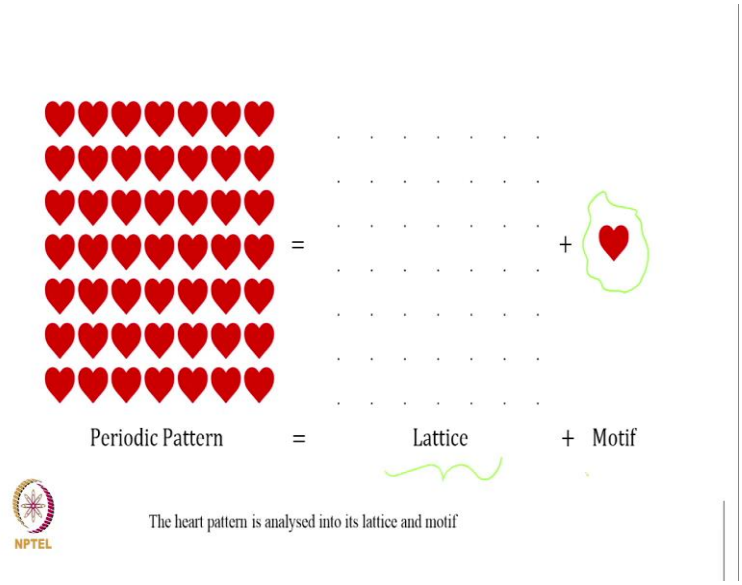

So, the pattern was there, and we extracted the lattice, from lattice if I want to go back to the pattern, I have to know what is being repeated. So, that is an additional information, that information is not in the lattice. That is why for the pattern, we require both lattice and the motif.

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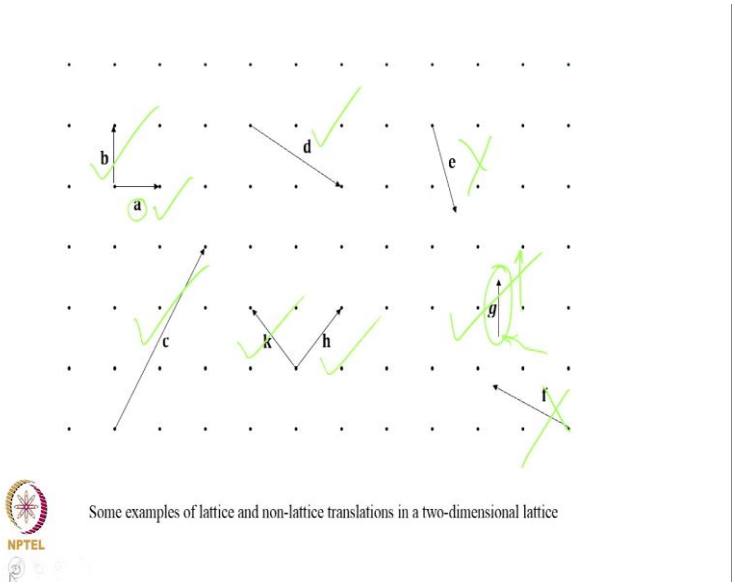

Some examples of lattice and non-lattice translations in a two-dimensional lattice

Professor: Rajesh Prasad: So, let us look at some of these lattice and non-lattice translations. We talked about yesterday that in any given lattice, if I have vector from one lattice point to another lattice point like this vector a connecting to nearby lattice point that said lattice translation. So, this is a lattice translation, b is also a lattice translation. What about c? Lattice translation, d keep saying yes or no. So that I know that you are with me, e?

Students: No.

Professor: Rajesh Prasad: e no, F?

Students: No.

Professor: Rajesh Prasad: g?

Students: Yes, yeah.

Professor: Rajesh Prasad: I am hearing yes as well as no.

Students: Yes.

Professor: Rajesh Prasad: Yes, why? Because vector wise which although I have not drawn it from lattice point to lattice point, but vector wise it will connect a lattice point to lattice point if I draw it from a lattice point only thing only mistake this vector was doing that it was not starting from a lattice point. But we know that vectors are translatable vectors are not fixed, we are talking about free vectors. So, this vector also qualifies as a lattice vector, k is also a lattice vector h is also a lattice vector.

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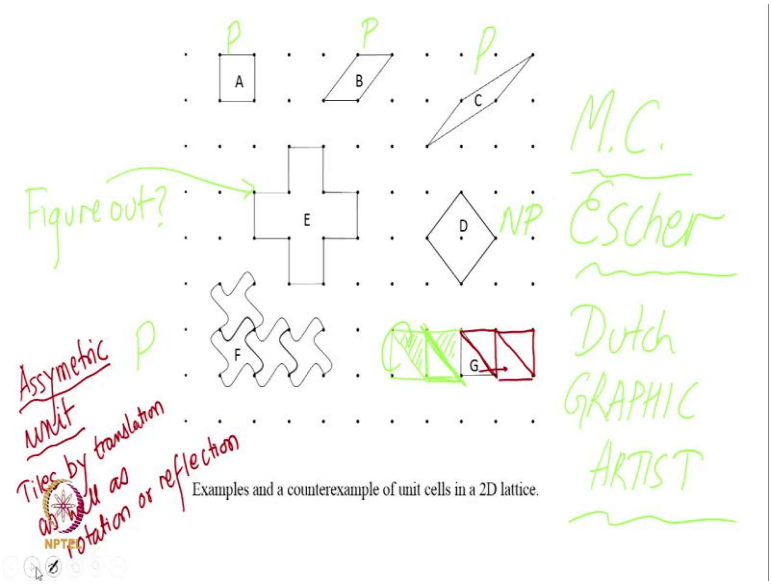

Good. Now, let us look at some examples of a unit cells, which we looked at yesterday. So again, you tell me, whether it is the unit cell and whether it is primitive or not primitive. So, is it a unit cell? Yeah, so a primitive unit cell. So, let me write this as P, it is still primitive. What about both are primitive. What about their size? Which is a smaller? Area wise both are same.

Who says so? Maths and what is the theorem base into height I like better cross product is also right. But why go to the complication? So, parallelograms with same base and same height will always have same area triangles with same base and same height also have the same area. So, that simple theorem makes them having the same area.

So, even sometimes when feels that there are infinitely many unit cells, there are infinitely many unit cells because there are so many different sizes of non-primitive unit cell but primitive unit cell is unique, no, primitive unit cell is also infinitely many you can keep having the same volume in 3D or same area in 2D but they still have different, different primitive unit cell in terms of their shape. C? Primitive D? Non-primitive. E? Primitive, non-primitive, not unit cell?

Students: Not a unit cell.

Professor: Rajesh Prasad: What was the definition of unit cell?

Students: (())(7:10)

Professor: Will it tile or will it not tile?

Student: It will.

Professor: it will tile it.

Student: It will overlap.

Professor: Okay left as an exercise will not answer. F? Definitely not, it is not straight edge.

Students: Not a unit cell.

Professor: Will not tile?

Student: primitive.

Professor: It will tile? That is a primitive unit cell who said that it should have a straight-edges and that is what the artists use. And one of the greatest artists in this field, we will look at his artwork sometimes M.C. Escher, a Dutch artist, Dutch graphic artist, very famous in Google, you will find thousands of things. And one of the things he was famous for was for creating periodic art. So, his art is having translational periodicity for one set of his art not everything. One set of is a he means he wanted to play with all kinds of periodic, but his periodic, if you make it of a square or rectangle who will buy your art.

So, his figures were birds, lizards, devils, demons, angels, all sorts of figures, which will be repeating and we will be fitting exactly together. So, they are also unit cells, his figures are unit cells you can find but with curved boundary, so you can curve the boundary and you still get the unit cell and you still have a reputation. D? This will not tile and because if I start repeating also.

I find that I am leaving some gap. This, because I need this triangle also to fill and this triangle is being left out, I can get this triangle by rotating this triangle or maybe reflecting in this edge. But that is not an allowed operation in the definition of unit cell. Unit cell should repeat by translational symmetry.

Later on, we will see there is another crystallographers do like this kind of thing also, that it starts with a smaller region and allow to reflect or rotate to fill their space that has a different jargon, I will share it with you, but we will look at it in detail later. That is called asymmetric unit, asymmetric unit. So, asymmetric unit tiles by, tiles by, translation as well as rotation or reflection that is allowed.

If that was allowed, then this triangle will qualify in that definition that I not only translate, I reflect it in this line, then I get this triangle. And then I translate, so I get this triangle and then I translate the green triangle, so I get this triangle then I will start filling this space. So, if rotation and reflection both are allowed, G will qualify, but then it will be a representative of asymmetric unit not off unit cell. Unit cell, the limitation is that it has to fill by translation.

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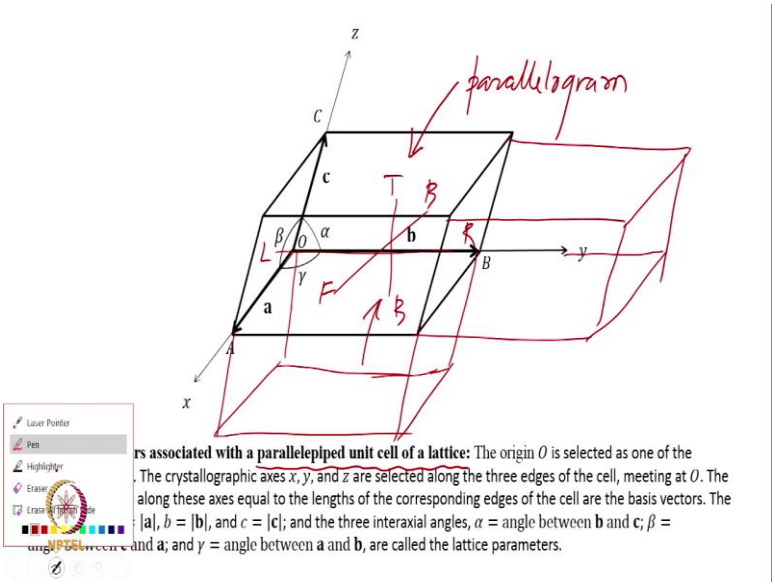
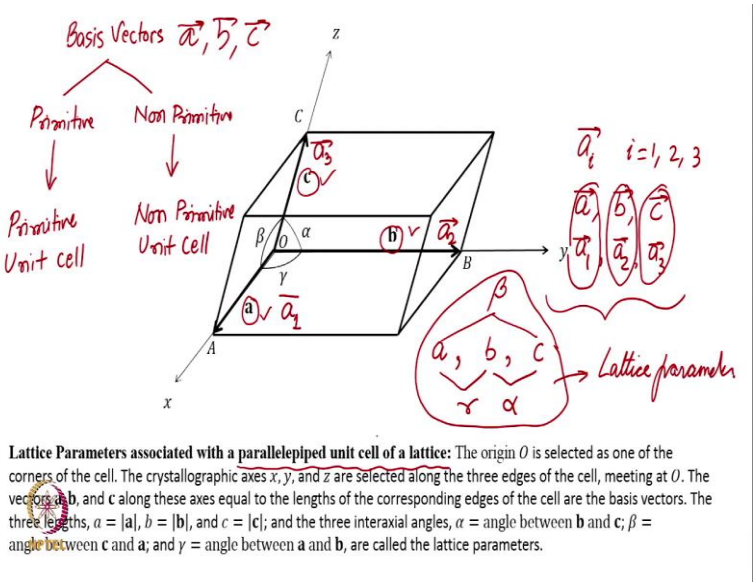


rs associated with a parallelepiped unit cell of a lattice: The origin O is selected as one of the . The crystallographic axes x, y, and z are selected along the three edges of the cell, meeting at O. The along these axes equal to the lengths of the corresponding edges of the cell are the basis vectors. The $|\mathbf{a}|$, $b = |\mathbf{b}|$, and $c = |\mathbf{c}|$; and the three interaxial angles, α = angle between $\mathbf{b}$ and $\mathbf{c}$; β = and $\mathbf{a}$; and γ = angle between $\mathbf{a}$ and $\mathbf{b}$, are called the lattice parameters.



Lattice Parameters associated with a parallelepiped unit cell of a lattice: The origin O is selected as one of the corners of the cell. The crystallographic axes x, y, and z are selected along the three edges of the cell, meeting at O. The vectors **a**, **b**, and **c** along these axes equal to the lengths of the corresponding edges of the cell are the basis vectors. The three lengths, $a = |\mathbf{a}|$, $b = |\mathbf{b}|$, and $c = |\mathbf{c}|$; and the three interaxial angles, α = angle between **b** and **c**; β = angle between **c** and **a**; and γ = angle between **a** and **b**, are called the lattice parameters.

In 3D, it was very nice to draw in 2D and we were playing with the rhombuses or parallelograms or even some odd shapes we saw, but in 3 dimension one of the standard unit cells is a parallelepiped, parallelepiped unit cell. So, parallelepiped you are familiar. Three parallel segments, three sets of parallelograms. So, each face is a parallelogram. And there are a pair of parallelograms which are parallel so that top and bottom left and right, and front and back.

So, this is our parallelogram unit cell. Parallelogram, what is the beauty of parallelogram unit cell? So, it will always tile the space if it is repeated by translations equal to its edges. So, if I go in this direction, I translate by B, I get the next parallelogram. In the bottom direction if I translate by minus C, I get that parallelogram. So, it will start filling this space. So, it is a unit cell parallelogram, parallelepiped are unit cells and that is the standard unit cell usefully used in crystallography.

So, although by definition of unit cell and particularly in the example of 2D we just saw that variety of unit cells are possible even with curved boundaries and also in 3D also you can imagine. And yesterday we did see one known parallelepiped unit cell what was that? The Voronoi cell of the BCC that was not parallelepiped but that is a unit cell.

So, 3D also it is possible to have shapes which are different from parallelepiped, but parallelepiped seems to be simple and standard, so we try to use it most often than not. If some need is there we do use. So, in solid state physics, when we require Brillouin zone or Wigner Seitz cell we deviate from parallelepipeds. Then this convention you know, one of the edges is called a, so, that is the basis vector.

So, now, these are the basis vectors a, b, and c and for any given basis vector either primitive basis vector. So, yesterday we saw that we have primitive basis vector basis vectors. We had primitive and non-primitive and if we make a parallelepiped out of a primitive basis vector, we get a primitive unit cell, primitive unit cell. If we make a parallelepiped out of non-primitive vectors, non-primitive basis vector.

We get non primitive unit cells. And the standard convention is to call one of them a, b or c or sometimes in more mathematically oriented discussion sometimes it is better to use a1, a2, and a3 because then you can use index so, for example, you can say ai, i is equal to 1, 2, 3 so, that will represent all the three basis vectors whereas, in the case of a, b, c you will have to write all three a, b, c.

So, sometimes we will use both we will use a, b, c also and we will use a1, a2, a3 also, a is, for a1 is for a, a2 is for b, and a3 is for C. And then the angles also are required because edge is alone will not define the shape of the parallelepiped, they can these vectors can have different angles. So, the angle, well, if you give them as, no I am making a mistake, if you give them as vector you have totally defined them because vector has both magnitude and direction.

So, there is no, no confusion if you are giving them as vectors. But sometimes you want to play with the scalars. So, instead of giving the vectors we want to give the magnitude of the vector so, instead of giving vector a, we give the magnitude a, magnitude b, and magnitude c. So, if we give only the magnitude these three magnitudes, then the shape is not fully defined, because, the angles between these magnitudes can be different.

So, we need to give angle also and the notation or convention is that alpha is the angle between b and c. So, see a, b, c, and alpha, beta, gamma so, b and c we leave a. So, whatever we are leaving we are converting that into the Greek sequence. So, b, the angle between b and c, a is left out alpha. Angle between a and b, c is left out gamma. Angle between a and c, b is left out beta.

So, that convention is used. So, instead of three vectors, if you give these six numbers, then also you have defined the unit cell size and shape. So, this is what is called so, a, b, c will be called the basis vectors a, b, c, as a basis vector, whereas, the length and the interaction angle those six numbers are called the lattice parameters.

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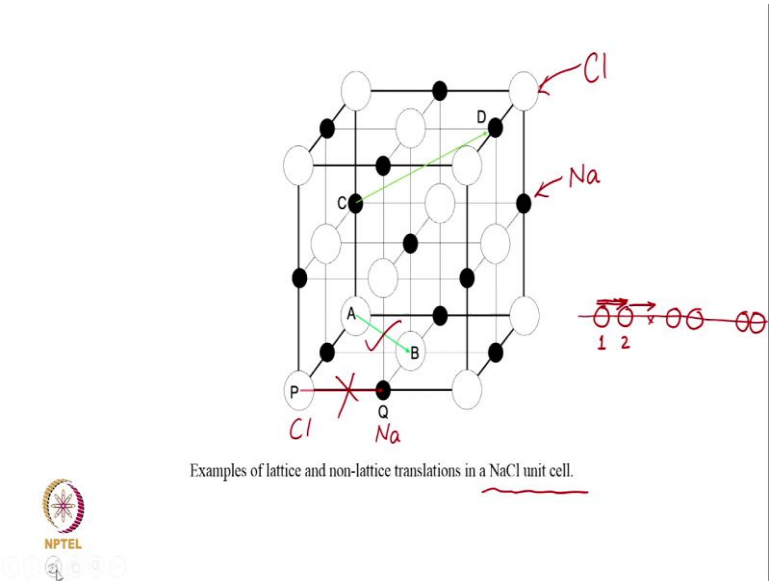

Examples of lattice and non-lattice translations in a NaCl unit cell.

So, let us look at some lattice and non-lattice translations here So, is P Q a lattice translation? This is a sodium chloride unit cell, it is written here sodium chloride unit cell. So, you can assume these to be chlorine and these will be sodium. So, is P Q a lattice translation?

Student: No.

Professor: No, why not?

Student: (())(20:26)

Professor: Takes me from a chlorine to a sodium. So, does not take me to an equivalent site. Equivalents require that I go from chlorine to chlorine. So, twice this vector will be a lattice translation, but this vector is not a lattice translation A to B. Yes, this is not, this is yes. C to D? Yes, you have to look a little carefully, it may not always be that if chemically same

atoms or ions are being connected that has to be a lattice vector, we will see examples. Sometimes chemically same elements also may be locally in different configurations.

So, they may not be forming an identical site, I think yesterday I tried to give you a 2D example, if I remember, that we have chemically identical atoms even 1D, not even 2D, 1D example. So, if in 1D we are going like this. So, all are same element, but if I go from here to here, that is not a lattice translation, because these two are not equivalent atoms they have different neighbourhood.

How they have different neighbourhood? Both have one neighbour each at the same distance. So, they have different neighbourhood because if I go towards the left, if, sorry right, if I go towards the right, if I go in the positive x direction, I find a neighbour for 1 but, if I do the same thing for 2, go in the positive x direction in by the same distance I end up somewhere where there is nothing.

So, 1 and 2 do not have identical neighbourhood. 1 has a neighbour on its right 2 has a neighbour on its left. So, this right left inversion also is noticed when defining the translational equivalence. So, C to D is also a lattice translation in this case, you can verify a little bit more carefully.

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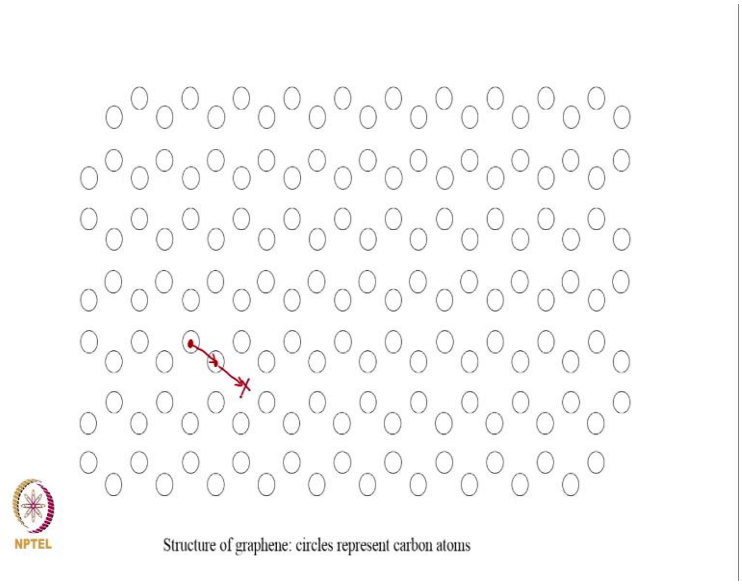

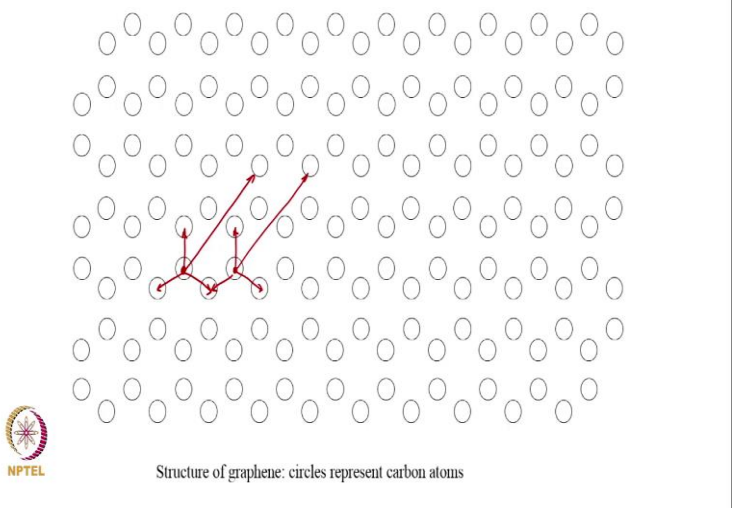

Structure of graphene: circles represent carbon atoms

We also saw yesterday graphene is a nice 2D example. And if we select any particular carbon atom as my origin and then I start thinking what is the lattice? How do I extract the lattice of this graphene structure? Then I think this is carbon and this is carbon. So, I can make a lattice like this, but then I find that then this will be defined as a lattice translation and this atom also should have a neighbour displaced by the same vector, but that is not true, that is not true.

So, this does not become this equivalent as a lattice point. But if I now look at this, if I now look at this, this is exactly the same environment. So, this has a neighbour here this also has a neighbour here. This has a neighbour vertically up, this has a neighbour vertical, this has a neighbour here anyway and not only local neighbours, far off neighbours should also be the same these are your neighbours there, this is also neighbour by the same vector.

So, in the entire pattern, you have to look at the entire pattern. Usually, we do not look at the entire pattern and we look locally because the periodicity guarantees, but means one has to be clear about that thing in mind that its repetition or equivalence with respect to the entire pattern and not only with the near neighbour or nearest neighbour also.

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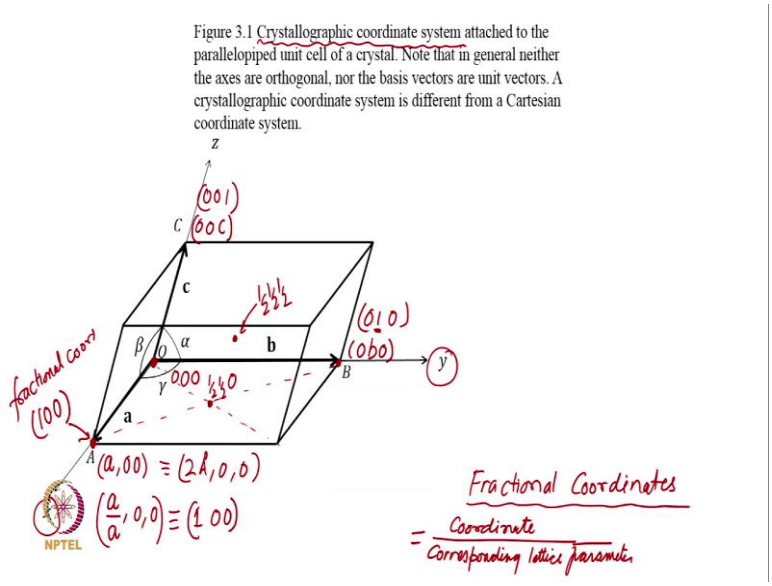

Now, this the basis a, b, c, gives you a what is called a crystallographic coordinate system very, very important concept. Important simply because it is not necessary and that is why the name crystallographic is being used, that it need not necessarily be Cartesian coordinates system with which we are familiar and that is the major confusion which happens in doing crystallographic calculation or this transition.

So, in crystallographic thinking our unit cell our a, b, c and alpha, beta, gamma defines my coordinate system, I am no more Cartesian. So, along a is my x axis along b is my y axis. So, the angle between x and y axis is gamma, whatever that gamma is. 120 degree what hexagonal crystals. Fine, I will live with that. I will not insist that the angle be 90 degree.

And similarly, whatever the length a and b be in Cartesian we say all are unit vectors all are equal and all our unit here neither we are saying that they are equal nor their unit. Whatever a is 1.3 angstrom, b is 2.5 angstrom, c is 4.393 angstrom, fine, I live with that. So that is what is a crystallographic coordinate system, because why?

Why crystallography means why take such a crazy coordinate system as against the nice beautiful well established and completely familiar Cartesian coordinate system? Because you will quickly see that actually Cartesian will not give you such nice coordinates for what we are interested in and that is the lattice points as the crystal coordinate system will give because we have selected a, b, and c to be lattice translation.

So, if I go from here, let us say. So, origin obviously has the coordinate o, o, o, and then there is a lattice point, there is a lattice point at a because a is a lattice translation. So it is it should take me from a lattice point at the origin to another lattice point at a. So, this is also a lattice point, what is its coordinate a, 0, 0. And what will be the coordinate of b? 0, b, 0. Here itself you are seeing the beauty of the crystallographic coordinate system.

Then, there is something called fractional coordinate. Fractional coordinates to simplify it further. We say that, why call it a, 0, 0, call divide the first coordinate by a, so, a by a, 0, 0, which becomes 1, 0, 0. So, call this point 1, 0, 0. So, 1, 0, 0 is the fractional coordinate. So, suppose a was 2 angstrom, then a, 0, 0 was 2 angstrom, 0, 0. But I will call it 1, 0, 0, so 2 angstrom is lost, 2 angstrom is lost, but that I am supplying separately by saying that I know what is the lattice constant.

I have kept that data separately and secretly that I know I know my a, b, c. So, even if you call it 1, 0, 0, I know that it is actually a, 0, 0, 1 times a. So, this will also become 0, 1, 0 I know that one is in the second place, so 1 time b and this will become 0, 0, 1. So, I will say it is one time c because 1 is in the third place. So fractional coordinate is coordinate divided by the corresponding lattice parameter, is equal to fractional coordinate.

So, idea of fractional coordinate is fine? Another beauty of fractional coordinate. Suppose I have something at the centre of this face, face centre, we have face centred lattices. We suppose there is a lattice point at the face centre also what will be its coordinates? half of zero. Suppose, I change the angle gamma to gamma by 2, what will be the coordinate of the face centre?

We still half half 0. So, half of 0 blindly I know is the centre of the bottom face of the unit cell. You do not have to tell me a, b, c, alpha, beta, gamma. So, that information is quickly transmitted, how hard will I have to work if you did not give me this fractional coordinate and gave it in terms of a, b, c, and even worse gave it a Cartesian system where the crystal was let us say triclinic.

Similarly, the body centre will become, half, half, half, irrespective of the unit cell shape do not think that half, half, half is the body centre of cubic unit cell, but what will happen in the triclinic unit cell? All these angles are something 39.6 and 122.9. So, I have to calculate the coordinates in the body centre? No crystallographers have made your life simple. Irrespective of the units that will shape the body centre has to be half, half, half.

So that is the crystal coordinate system for you. Very nice system developed by crystallographers.