Crystal, Symmetry and Tensors
Professor Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology, Delhi
Lecture 1a
What is Crystal?

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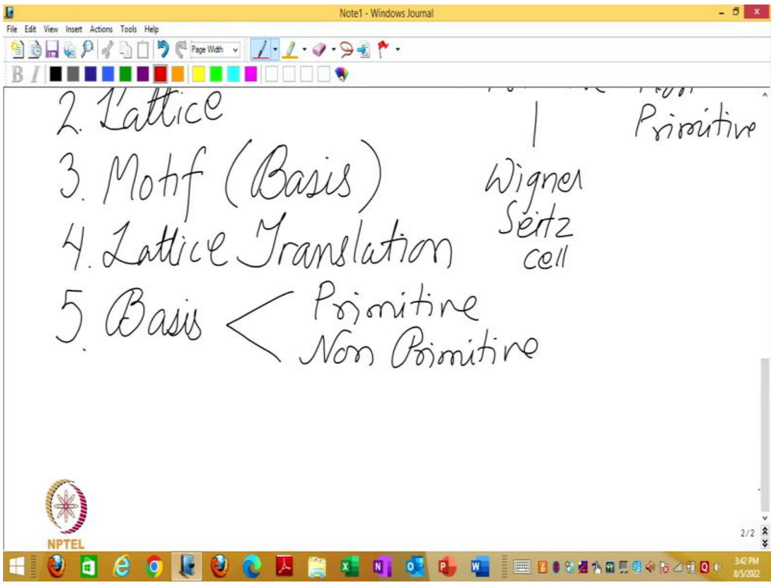

Welcome to Crystal, Symmetry and Tensors lecture 1. So, let us look at the topics which we will try to cover in this very first lecture. Although this is we want to go reasonably advanced level in this course with crystals and we want to let us say discuss point groups and space groups, coordinate transformations, matrices, tensors, and all that sort of thing.

But to begin with to bring all of you on a level playing field because you are from different background, somebody from mechanical somebody from physics, chemistry, all of you must have studied crystal, I am quite sure, in some part of your curriculum, because nobody can get away doing science or engineering without touching crystal.

But the idea of this course is to take you to the next level in thinking about crystallography and symmetry but we will begin right at the beginning, where the beginning will be very, very basic. So, that will be the first week, you can think of it as a review or review for those who have definitely done it and remember it and even if you have not done it, if you think I do not think anybody can say that I have not done it, because this is there or even in the school curriculum. In NCERT curriculum, I know 11, 12 people do solid state chemistry and crystals and these kinds of things. But let us since our concern is concern is Crystals, since our concern is Crystal.

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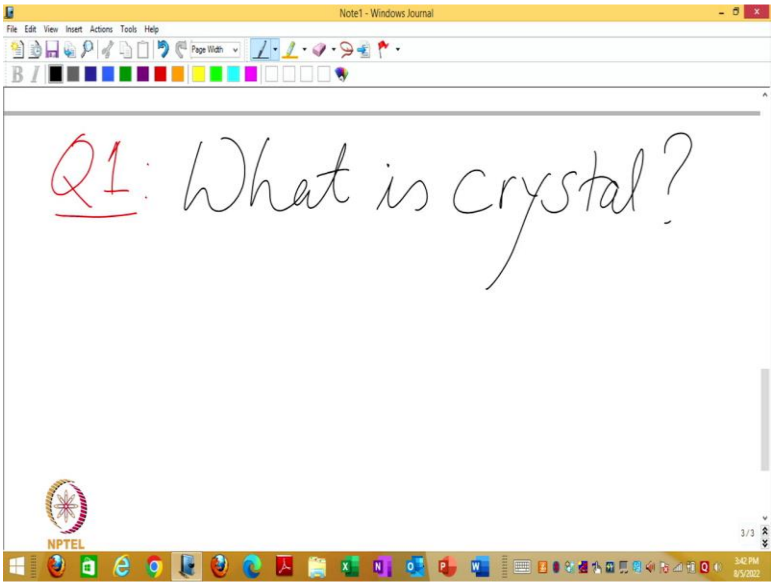

So, let us begin with really at the beginning. So, let us begin with let us call me question 1 what is crystal? Define, define crystal if somebody asks you to define crystal, how will you define?

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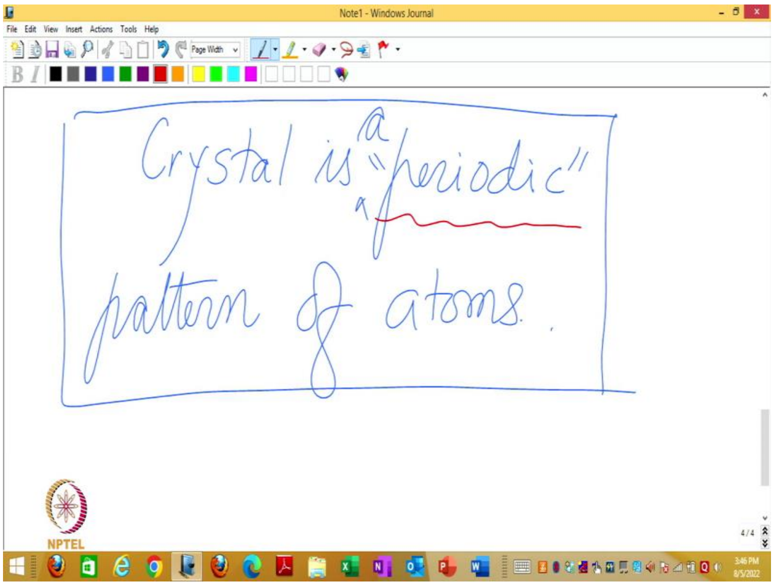

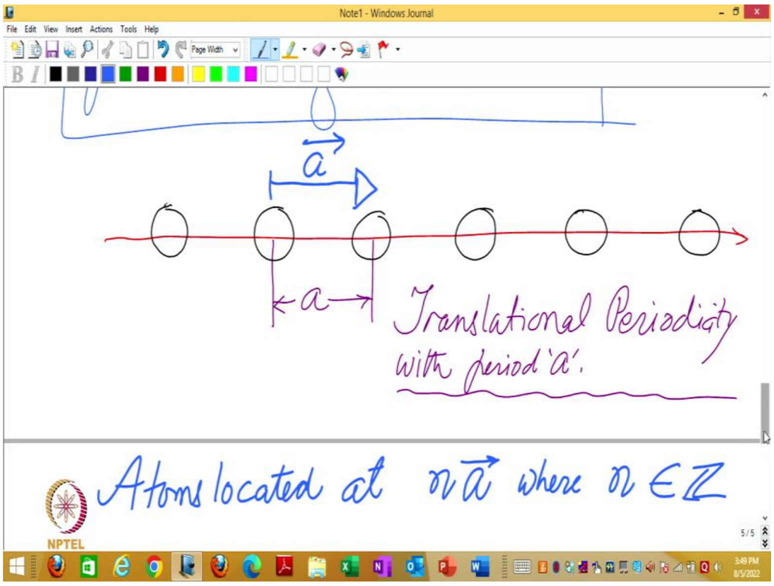
Note1 - Windows Journal
a
Translational Periodicity with period 'a'.
Atoms located at n a where n ∈ Z
NPTEL
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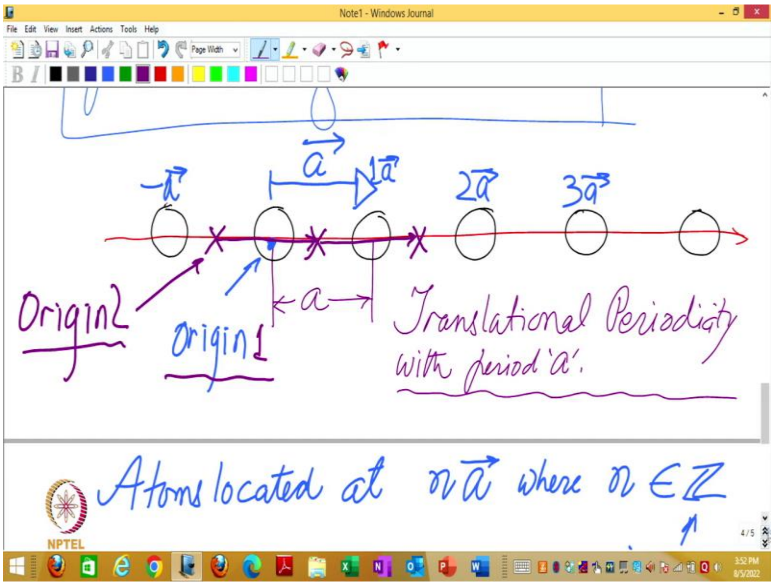
Note1 - Windows Journal
-a
a
1a
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Origin1
a
Translational Periodicity with period 'a'.
Atoms located at n a where n ∈ Z
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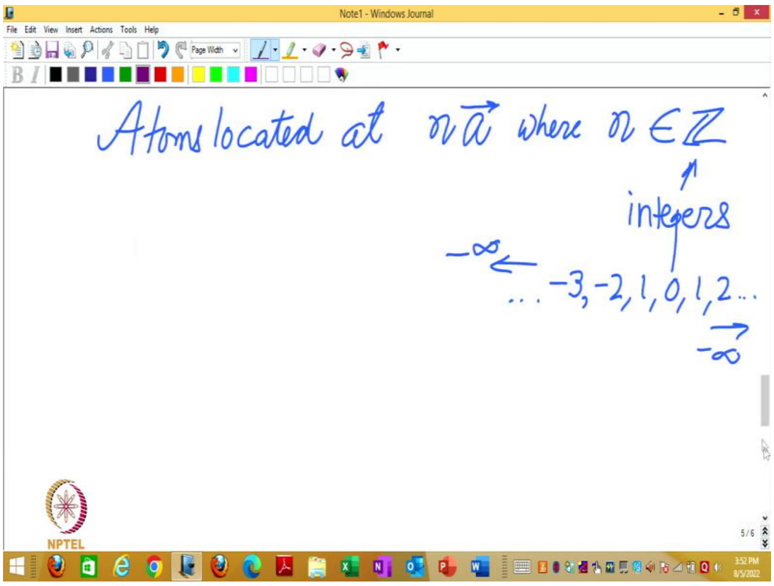
Note1 - Windows Journal
Atoms located at n a where n ∈ Z
integers
-∞
... -3, -2, 1, 0, 1, 2 ...
-∞
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So, let us put this this way. The same thing what you have said I am again rewriting. So, crystal is periodic periodic pattern of atoms, so this is our definition. Regular arrangement is fine, but regularity can be of many different types, periodic is a specific kind of regularity. So, that is important, to say periodic just saying regular is not that good a definition and similarly ordered, ordering also is of different kinds ordering also is of different kind and but periodic again makes it a little bit more specific, a little more clear. So, periodic is important.

So, let us look at some examples. So, let us begin with again let us begin with beginning let us not go into three dimension, let us keep ourselves into one dimension, and let me try to draw something like one dimensional periodic arrangement of atom or crystals are three dimensional but within crystal there will be rows of atoms which are periodic. So, those rows you can consider as one dimensional periodic arrangement of atoms one dimensional periodic arrangement of atoms.

So, periodicity means it is repeating at equal distance. So, if I take the distance to distance center to center distance a it is repeating at distances a at each distance a if I move each distance a either forward or backward, I find an atom and I find the same atom. So, it is having translational periodicity we will say that it is having a translational periodicity periodicity with period ‘a’.

Now, this you can you can bring in vector here and say that the translational periodicity is represented by you can draw a vector of length a and direction pointing to the right you could have taken direction pointing to the left also does not matter, because we will say that there are atoms located, located at end times the translation vector a where n is an integer so, that means it can be anything between minus infinity let us say minus 3 minus 2, 1, 0, 1, 2 to both direction it can go negative minus infinity and positive infinity.

That is why I said that you the direction of the arrow, initial selection of the sense of the arrow is not that critical, because I am allowed to take both positive and negative n so, I am actually going with so this is 1a, I will reach here by 1a I will reach here by 2a, I will reach here by 3a I will go backwards also, because I can go minus a or minus 1a.

So, translational periodicity is represented by translation vector. So, one dimensional translational periodicity requires only one vector. And the vector the translational symmetry vector does not have any origin. Although I seem to be saying that we are starting so, I have selected when I wrote 1a, 2a I selected this as my origin because this was 0a.

But, I could have selected some other origin also. Even if I let me select a point in between the two atoms then also from here also I can get go to a vector a and come to a translationally equivalent position if I was in the middle midpoint of two atoms and I shift by a I again I am midpoint between two other atoms which is translationally equivalent and again midpoint of two other atoms.

So, a starting point is not really important, let us say this is origin 1 this is origin 2, but both will give me the same translational periodicity. So, choice of origin becomes sometimes very, very important. And in the crystallographic communication, it becomes important to tell to the listener or to the audience or to your reader that what is your origin otherwise, the description one with origin 1 will say I have atom at my origin. Origin 2 will say I do not have any atom at the origin.

So, everything that they are talking about two different crystal structure one has atom one does not have atom but it is actually the same crystal but with different choice of origin. So that we will discuss more a detail. There is just a hint. That origin choice is also quite important.

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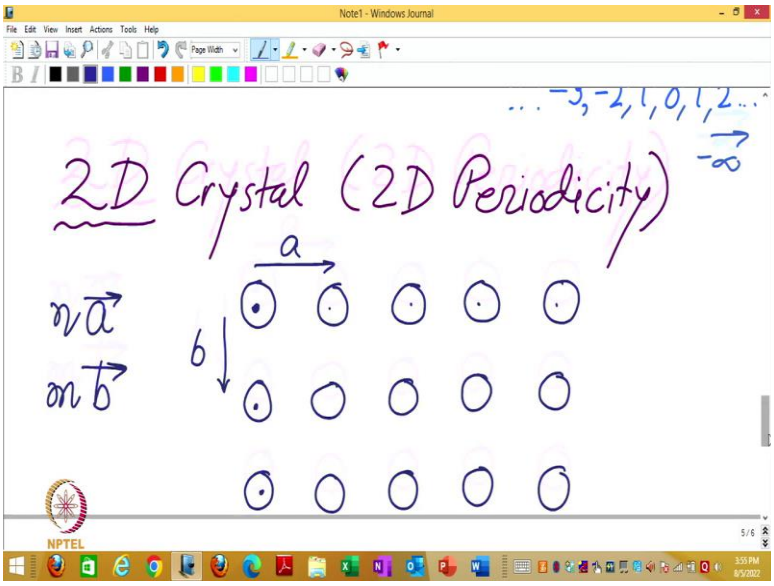

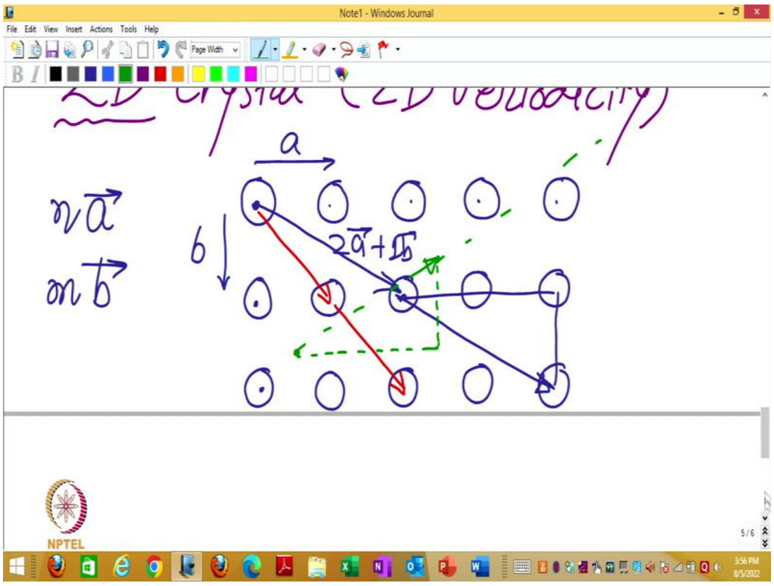
Note1 - Windows Journal
a
b
nā
mb⃗
2ā+1b⃗
NPTEL
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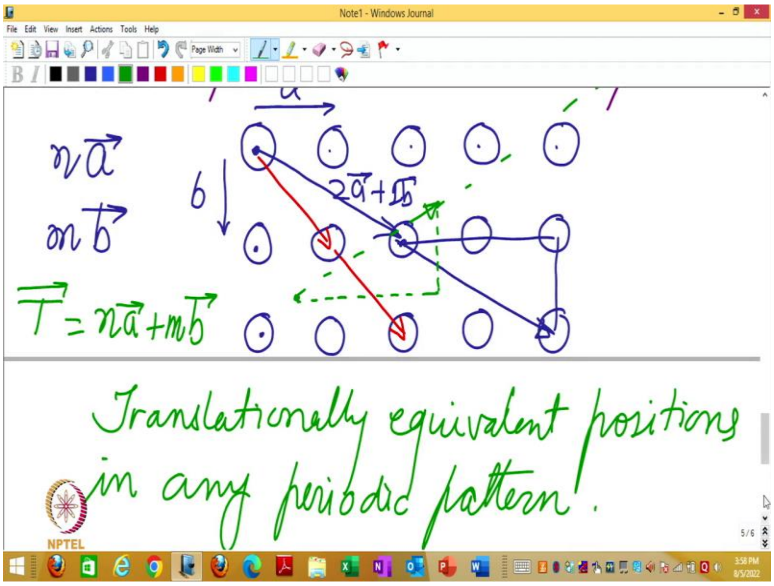
Note1 - Windows Journal
nā
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2ā+1b⃗
T⃗ = nā + mb⃗
Translationally equivalent positions in any periodic pattern!
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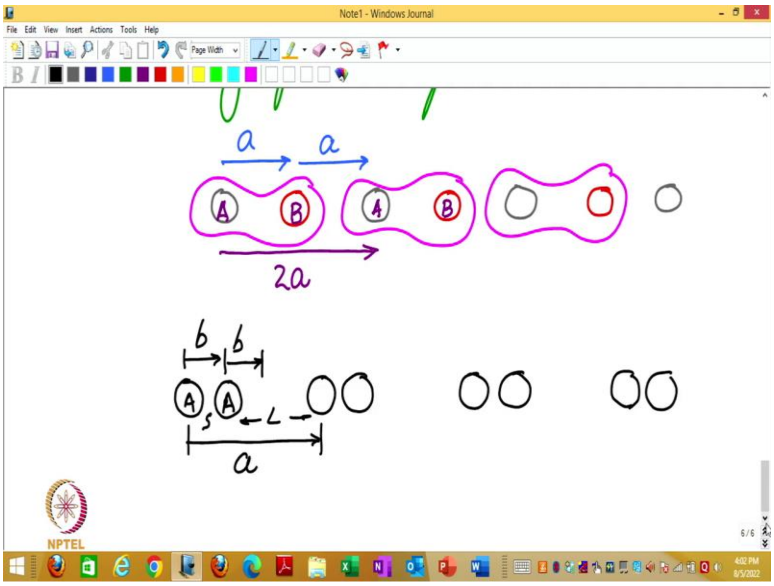
Note1 - Windows Journal
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Yeah. So, now let us look at 2d 1d was very very simple. So, let us look at the two dimensional example 2d crystal here we have real examples also for example, you know graphene nowadays. So, graphene can be considered as a two dimensional crystal having two 2d periodicity, but, graphene is a little complicated, we will see what the complication is. So, let us say create something much more simpler.

So, this is why this is one dimensional periodicity we have already seen we are shifting by certain distance a. But now, I decided to shift in the other direction also by some amount b not necessarily equal to a. Although I can keep it equal also but a little bit more generality I have made it b. So, from anywhere if I move n times a, from any starting point again maybe my starting point is center of the atom. So, if I move n times a, from any atom considered as origin I will again be on an equivalent atom.

Similarly, if I move b amount b m times b I still will be I will still be on the equivalent atom equivalent side, and if I go somewhere in that direction which was not my original periodicity direction that also happens to be periodic because now I have gone two time say this was 2a plus 1b and now, I further move 2a plus 1b from here 2a plus 1b again I go to an equivalent atom.

So, although we started with periodicity in two directions, it seems we have generated periodicity in many many directions infinitely many directions, because if I go this way also then, the same translation further keeps taking me to equivalent position and as I told you in the previous one dimensional example, if I choose a different starting point does not matter if I go let us say 2a this way and minus 1b this way. Again I come from center of square to another center of square. And if I keep doing that, I will keep getting in to equivalent positions.

So, there are translationally equivalent positions translationally equivalent positions any periodic no sorry, not periodic lattice we have not yet defined lattice. So, periodic pattern we just call it pattern. So, let us look at some little bit more. So here in both examples, all atoms were translationally equivalent 1d, all atoms were translationally equivalent 2d again all atoms were translationally equivalent.

So, here is the translation general translation you can write as T is equal to na plus mb. So, this takes care of all possible equivalent translations in this structure or this pattern. But let us try to make something, something different. Let us try to create, now does this have a translational periodicity of a, because by a although by a you get an atom, but now you get a different atom instead of black atom you get a red atom.

So, a is no more your translation (equiva) means translational periodicity of this structure, the translational periodicity of this structure becomes 2a. So, all atoms in this structure are not translationally equivalent. So, this is an example where the atoms are chemically different one is an atom A, one I am calling atom A, the black atom and another one atom B, the red atom.

So, it is easy to see that they cannot be by translation you cannot transform and A in to B by translation, by equivalent translation you have to go from A to A. So, this is a, so is this then a periodic structure with periodicity 2a, but then what is the thing which is repeating AB, AB the pair. So, in this case a pair AB is repeating.

Now, let us let us take yet another example. It is not necessary for atom to be chemically different. Suppose I have some molecule kind of thing two atoms close by. Again, if I move from here to here let us say by the bond distance b, I find an atom identical atom, but from here if I move by the same distance b, I do not find an atom. So, that means this right atom this one is not equivalent to the left atom, because left atom has a neighbor to its right at a distance b, the right atom does not have an identical neighbor on it is right at the same distance b.

So, they are not translationally equivalent, but if I translate all the way from here to here, then I get the periodicity. So, there in the previous example, since the chemical elements were different distances were the same, but chemical elements were different that may that broke the translational periodicity from A to B.

Now, although elements are same both are A atoms let us say. But, because of distance separation is changing from short distance to long distance between them, there is a short distance here and there is a long distance here. So, again that makes all atoms not equivalent and you have to move by this distance. So, let us try to take little bit more involved example. As I promised, let us make graphene.

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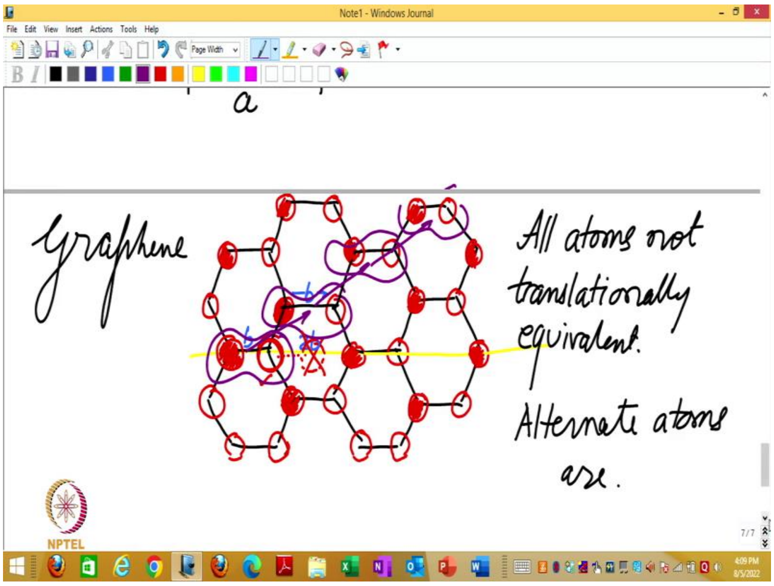

So, let us make graphene, graphene I need a hexagonal honeycomb. So, you have a hexagon neck like this hexagon tile is one of the interesting and simple tiles and on this on all the vertices of this hexagonal tile if you put an atom, carbon atom. So, I put one carbon on all the vertices carbon should have been black I think, but anyway I have drawn in red are all carbon atoms equivalent translationally.

Think about that why not, which are different and which are same. So, if you think of the hexagonal geometry and if the hexagonal edge length is a not let us not call this a let us call this b the carbon carbon bond length, let us call this b the carbon carbon bond length, then by hexagon you know that the diameter of the hexagon is two times its length this from your school geometry you can easily prove.

So, this is b this is 2b. So, if I think if I start focusing on the atom which I have shaded and then I say that whether this shaded atom and the other atom at the end of this distance b this one are they equivalent. So, this atom has a neighbor this one at distance b, but if I go the same distance from this in the same direction, I find a hollow there is no atom there.

So, the neighboring atoms are not equivalent. But if I go to the next neighbor here then this of course has another atom at near distance b in the same direction. So, neighboring atoms are not equivalent alternate atoms are equivalent. So, in the graphene in the graphene pattern so, I am now shading all the equivalent atoms translation equivalent in what sense, chemically of course, they are all equivalent chemically all our carbon or if you think your equivalent definition is that how many bonds it is forming.

Again all are equivalent all of them are forming three bonds. So, when I am saying that they are not equivalent, I am saying that they are not equivalent in a particular sense and that sense is translational equivalence that they are not translationally equivalent the neighboring atoms with alternate atoms are translationally equivalent. All atoms not translationally equivalent. Alternate atoms are.

So, the center of alternate atoms only will form the lattice that is bring us to the definition of the lattice that what is. So, we have defined crystal as a periodic pattern and we have seen that the thing which is repeating periodically can be one atom or more than one atom. So, here what is repeating periodically what can we say, yeah, two atoms because if I, if I say only the shaded atom then I will get only half the atom. So, I have to take a long shaded and unshaded atom that pair and then I think that that pair is being repeated periodically you can see in the structure, so from here, if I go here, to here to here, I keep getting identical pairs. So I can select a pair of atoms in this case.