An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
Prof. Ashish Garg
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

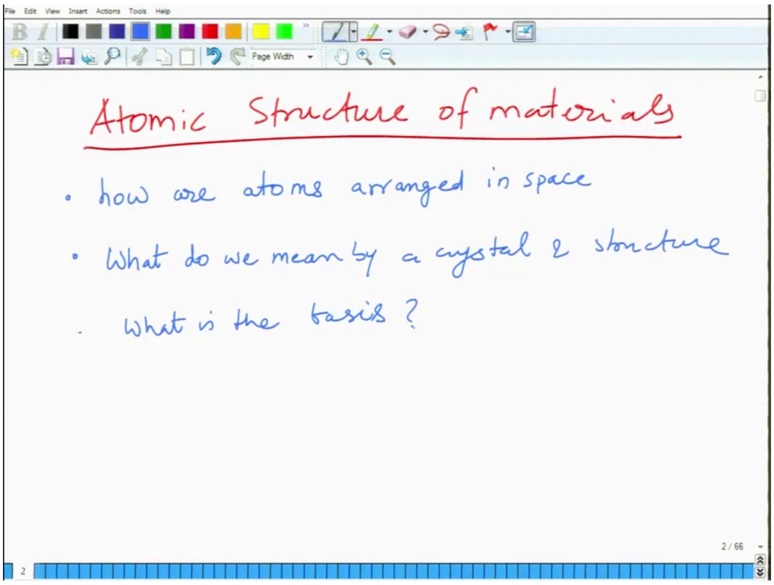
Lecture – 04

Crystal Structure: Lattice and Basis

So in the previous lecture we learnt about the fundamentals of bonding without getting into any quantitative treatment, we will do some quantitative treatment as an when we learn about those solids and their structures a little later in the course. So, for the sake of simplicity let me just brief that covalently bond energy is a function bond energy determines properties like melting point coefficient thermal expansion and elastic modulus and higher the bond energy higher the melting point higher the modulus it is going to be and lower the coefficient thermal expansion going to be now bonding is 1 factor in determining the structure of materials.

So, what is the 1 very important factor and this basically determines, so when you do calculations to predict the structure of materials you have to consider that particular aspect. So, now let us move on to the structure of materials by structure first coming from bonding we move to the atomic structure of materials. So, here in this lecture and onwards we will learn about what we call as a atomic structure of materials and the objective of this is basically to learn how are atoms arranged in space.

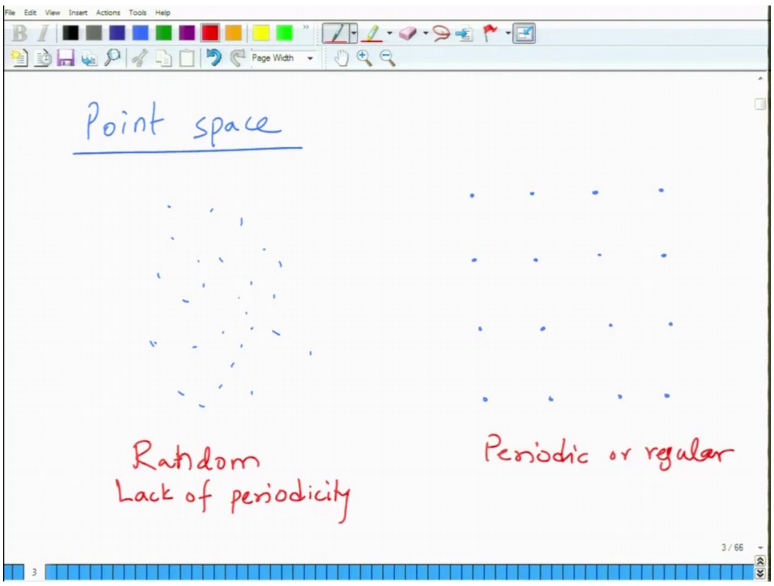
(Refer Slide Time: 01:42)



Of course, there is whole mathematics which is behind the structures, but will not get into those that mathematics right now ah.

So, how are these atoms arranged in space, what is the what do we mean by a crystal structure crystal and structure and what is the basis ok. So, before we get into this we first, so we know that since you have atoms they are connected by various bonds, but now the question is how are these atoms spaced in the in the universe or how are replaced in the space. So, before we talk of atoms we just start with random points and space.

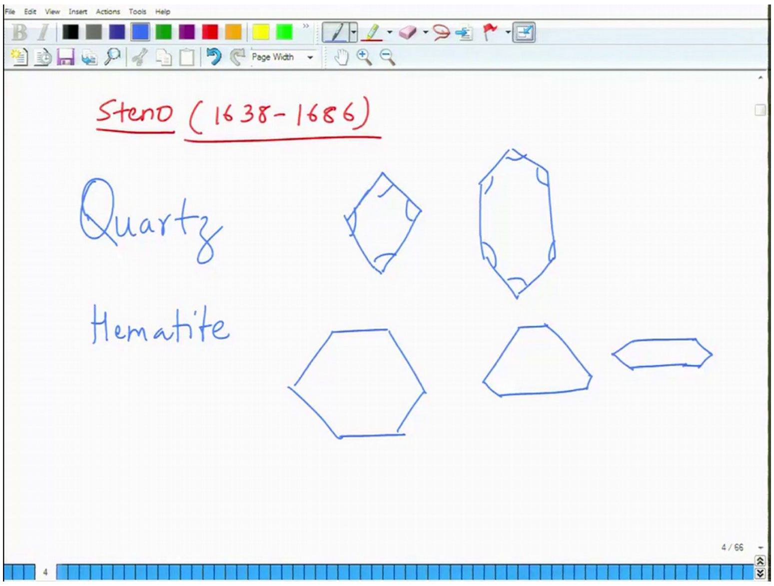
(Refer Slide Time: 02:21)



So, we just looked at first the points and space considers replace the atoms by points. So, there are various methods by which you can do that the points may be spaced like this or the points maybe space like that, these are just to illustrations there are various other possibilities.

So, in one situation you have a distribution which is random in this case what do you call it you will call it periodic or regular ; at least you can see a pattern there on the right side, but you cannot see a pattern here on the left side. So, here it is random without any periodicity you can say lack of periodicity, most materials in nature with the exception of few tend to have atoms arranged in regular fashion. So, when you look at the atomic structure you will see that the atoms are placed in space in a every regular pattern and where does where did I where did the motivation behind come from the motivation come from the works of some previous scientist; for example, there was a scientist called as steno ok.

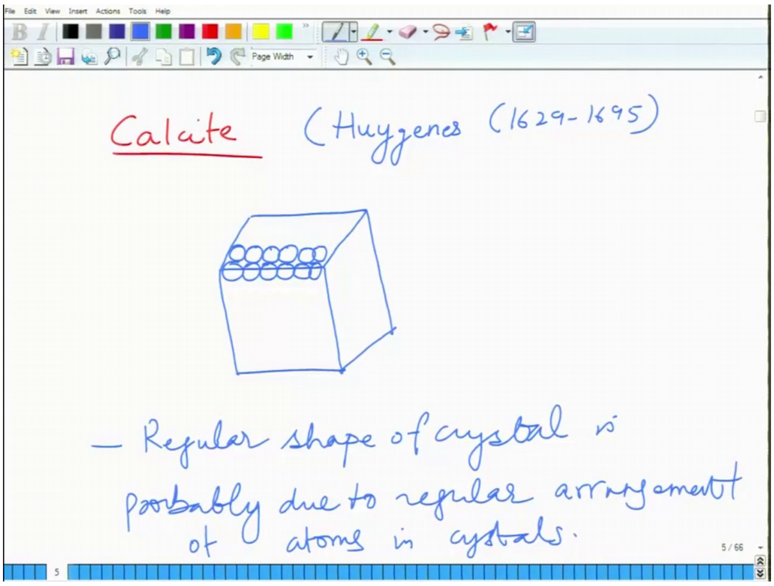
(Refer Slide Time: 04:00)



Steno was a sign scientist who lived between 1638 to 1686, you can see he only lived for very short time. He noticed he made drawings of things like quartz and he made drawings of things hematite and what he did was he made these kind of drawings ok.

He made these regular shapes, now these shapes there many of them he drew not only these, so I am going to draw only a few of them. So, he made the shapes because he observed that crystals they tend to have certain shapes and there is a constancy about of a phase angles some of these angles that you see here, they tended to have certain relations with each other you could put feed these angles into a mathematical frame work and get a order about these angles and there was relation between these angles. So, steno was the first 1 of the first guys to observe that crystals have certain geometrical patterns about them and the angles of phases and edges can have correlations.

(Refer Slide Time: 05:30)

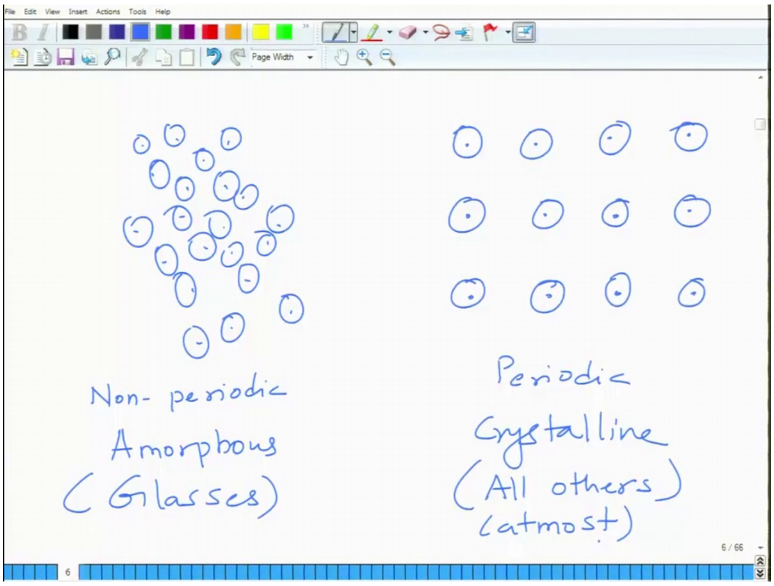


Then later on in noise] calcite crystals this was the work of Huygens ok, who was from 1629 to 1695 again people did not belong in those days only 66 years he lived.

So, calcite crystal for example, had a peculiar sort of geometry it have geometry like that. So, so this sort of geometry post trying to set that time to think that if a calcite crystal macroscopically can have such and such a regular shape then what must be about the atom sitting inside the crystal. So, perhaps it also because the atoms in this also sitting in a ordered fashion in something like that I am not saying it is exactly like that, but there must be some order about the atoms which are sitting inside. So, that is it is only because the atoms if the atoms are sitting inside in a regular fashion, the crystal itself would manifest in a regular shaped.

So, this was the underlying basis of why so you can say that first thought was regular shape of crystals, is probably due to regular arrangement of atoms in a crystals. So, these were some earlier indications of why atoms could be arranged in a periodic fashion in a space. So, that is where when I come back to again my picture. So, you have distribution like this.

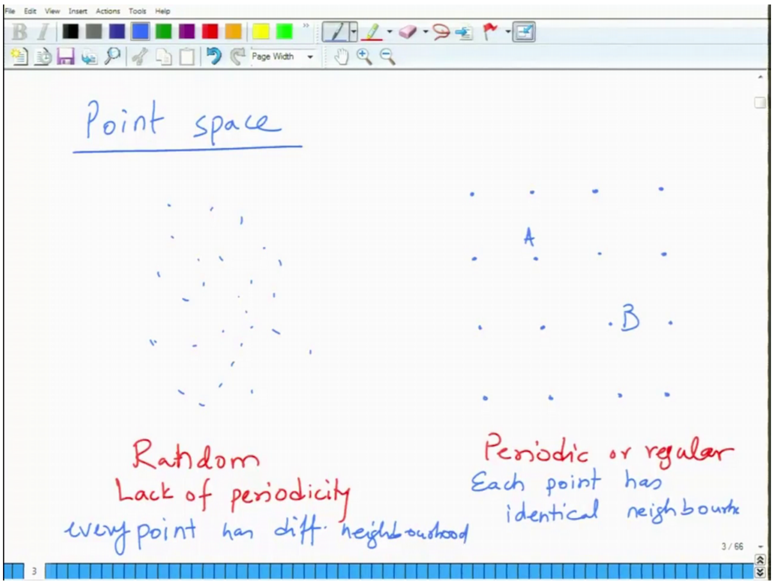
(Refer Slide Time: 07:38)



So, we replace the atoms with points and then of course, you have something like that. So, this is non periodic and this is periodic and if I put atoms here instead of points I make a crystal basically. So, in this crystal considering atoms as spherical in nature, so this would be has no longer in periodicity such materials are all also called as amorphous and the materials in which this kind of periodicity is there these are called as crystalline.

So, amorphous materials are typically things like glasses, but all other materials almost I would not say all of them, but almost all of them. So, all others almost are crystalline in nature, which have periodic arrangement of atoms ok.

(Refer Slide Time: 09:09)



So, in this case you had a random arrangement of points without any periodicity in the structure, here you have periodic or regular arrangement of points. So, in this case I call it that there is no, so every point has different neighborhood right, can I say that every point in this has different neighborhood is that a correct statement to make .

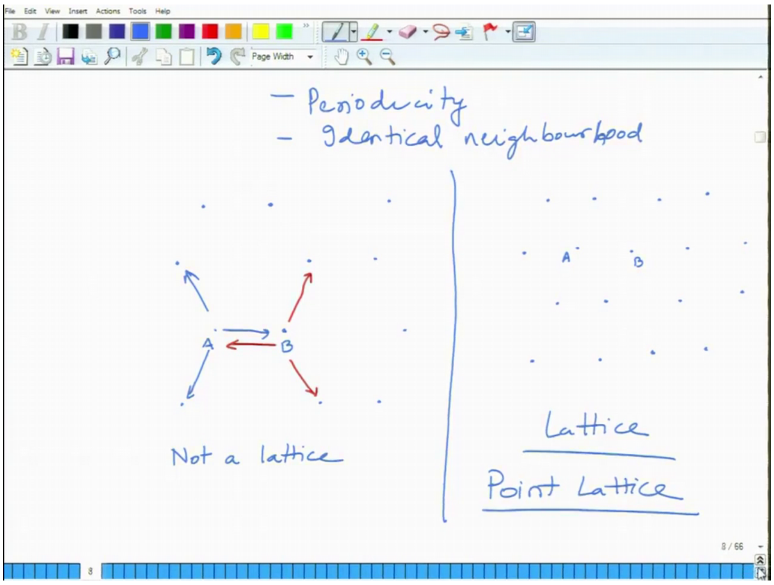
Student: (Refer Time: 09:45).

Because each point is randomly distributed in a space there is no correlations of lengths and angles and directions, as a result the if I look around myself there are 4 guys, if a certain 4 guys are in certain distance certain angles, but if another guy close to me looks at his surroundings he points at all there could be 5 there could be six and at different angles and directions.

Student: (Refer Time: 10:34).

So, the coordination number will be different ah, but coordination number is something which is defined by fix distances ok, in this case even the distance is not fixed. So, there is no fix coordination number here ah. So, every it is better body to say that every point has different neighborhood, in this case when you standard point a when you standard point b you see the same arrangement right. So, each point has identical neighborhood right. So, that is first thing that now let me make another structure which may look periodic in nature by still not periodic. So, let me let me draw something here.

(Refer Slide Time: 11:04)



Now if I let us say standard point A and if I standard point B do they have identical neighborhood this is a hexagon arrangement ok, this is hexagonal arrangement, it is I means it is a very precise here, but it is kind of hexagonal in nature.

Student: (Refer Time: 11:44).

For you have 1 neighbor on here another neighbor here another neighbor here, for b you have 1 neighbor here another neighbor here another neighbor here. So, number of neighbors are same, but is the arrangement of neighbors same it is not, for a you see 2 neighbors on the left at certain angle at certain direction and another neighbor on the right; in certain direction the distances are same, but the directions are different for b you see 2 neighbors on the right 1 on the left ok; it is kind of a mirror image but it is not identical. So, this is not a so let me now make another modification to this the modification is ah, so ok.

Now, let me put a point here, so you have a point A and you have point B do they identical neighborhood now.

Student: (Refer Time: 13:13).

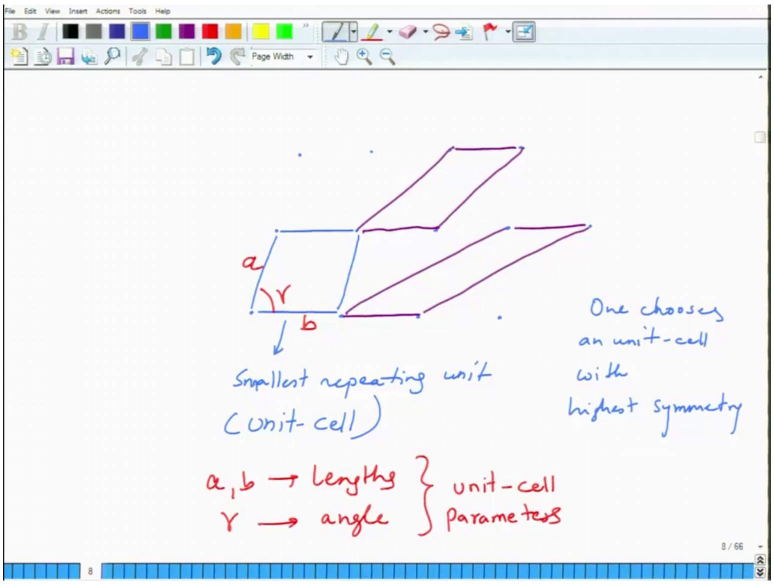
A and B both.

Student: (Refer Time: 13:15).

They are now have identical neighborhood. So, I would say merely having a periodic arrangement apparent periodic arrangement there is not fine the identical neighborhood is has to be obeyed. So, I would say this structure is not a lattice this is the lattice. So, by definition when point arranged themselves in a space in such a fashion, so that the arrangement is periodic and every point has identical neighborhood these 2 conditions qualify that arrangement as a point lattice. So, this is called as point lattice. So, that 2 definitions are periodic periodicity and identical neighbor.

So, these are 2 distinct in scenarios now let me ah, so once we defined a periodic lattice in this fashion let me draw a periodic lattice .

(Refer Slide Time: 14:38)

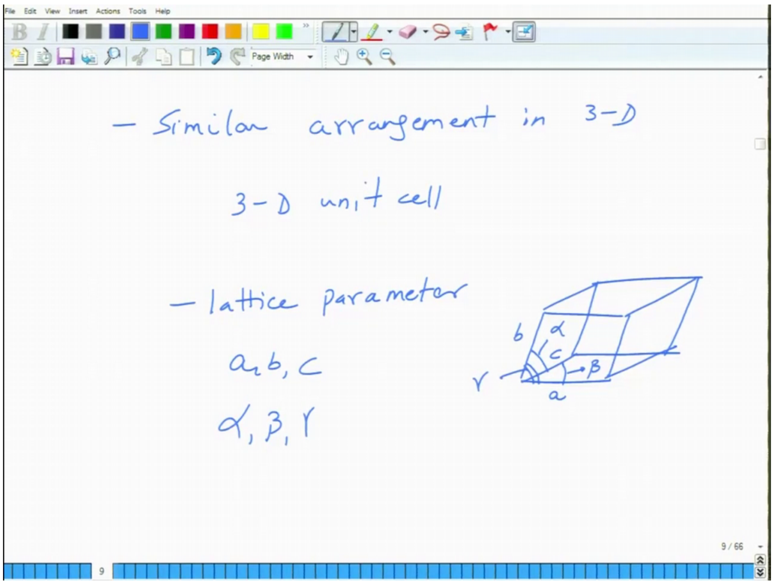


So, this is a periodic lattice in this periodic lattice I so I can draw a smallest repeating unit, this is the smallest repeating unit this is called as this is called as unit cell ok; however, let me and these and the sides of this unit cell are called as unit cell parameters. So, if this is A this is B this is gamma. So, these will be A B and so A Bare the lengths gamma is the angle between the 2 edges these are called as unit cell parameters.

Now, my question is the choice of this unit cell unique, I can also make a unit cell like that basically all you have to have a smallest repeating unit, this is also a smallest repeating unit it has a same ideas other 1. In fact, if you make this 1 here and if I put a point somewhere here this is also a valid unit cell. So, the choice of unit cell is not unique choice of units the unit cell these are all unit cells. So, which 1 to you choose you choose the one with the highest symmetry. So, that is why the concept of symmetry comes into picture.

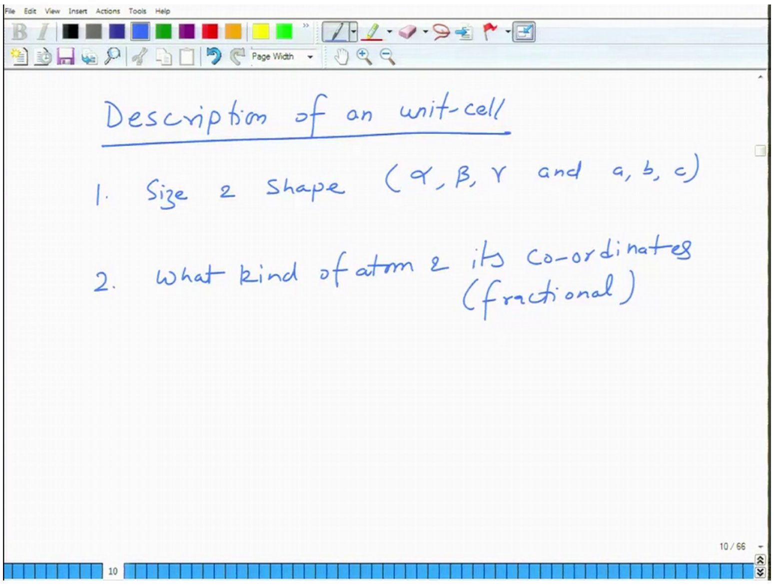
So, one chooses an unit cell with highest symmetry and we will see what is the meaning of this highest symmetry ah, as of now you can just assume that whatever looks symmetric to you is of that off with highest symmetry, but we will come the definition of the symmetry in a short while maybe perhaps in the next lecture. So, you can have similar arrangement in 3D similar arrangement in 3.

(Refer Slide Time: 17:41)



So, it will make a unit cell which is a 3D unit cell and in 3D you will have lattice parameters as a b c and alpha beta gamma. So, basically it will looks something like that a parallelogram all right; a b c and angles this is first angle this is another angle and this is another angle these are 3 angles. So, between a and b you will have gamma and between b and c you will have alpha and the beta. So, this is the periodic structure this will be a 3D unit cell of a material, so basically the unit cell requires few points for description.

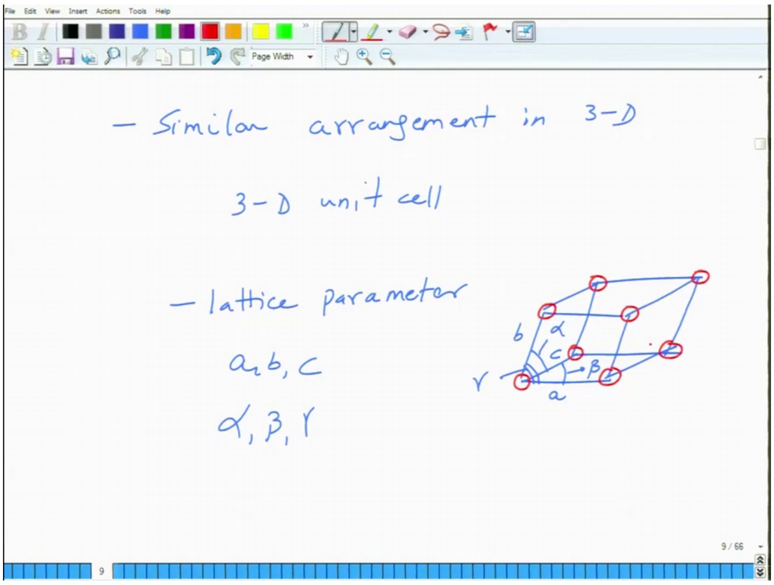
(Refer Slide Time: 18:46)



So, descriptive first thing you need to measure it is size and shape, size and shape is determined by alpha beta gamma and a b c, what is the other thing that you require now if you replace the points by atoms if you replace the point by atoms points are taken for the sake of convenience ah, because atoms can make it little complicated you may not have just 1 type of atom you may have different types of atoms.

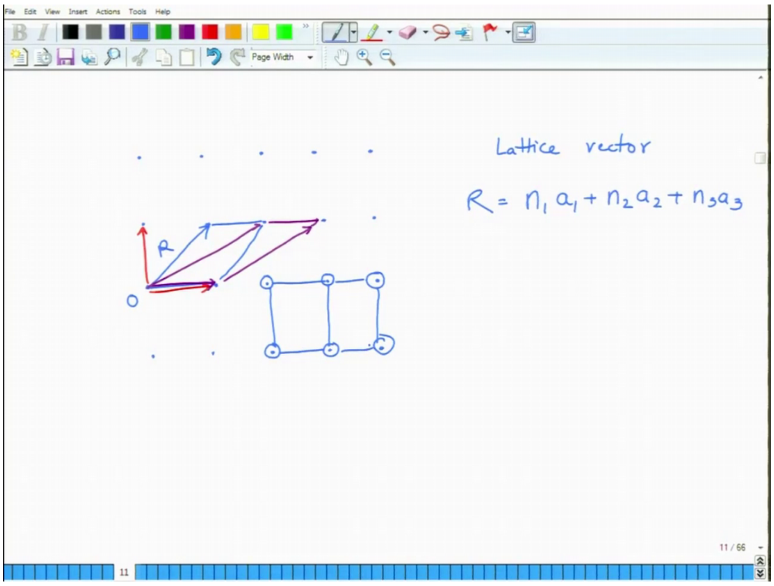
So, that is why we just begin with the point now let us say we replace the point by an atom and identical atom ok, then what we required is basically the what kind of atom and it is coordinates basically what we required is the fractional coordinates of the you can say the fractional coordinates of the atoms. So, these few things are required to specify. So, if I replace these points by atoms here.

(Refer Slide Time: 20:05)



So, these are all atoms, so to describe the unit cell you require these positions to be known now I have we have seen. So, a, b, c are the lattice parameters alpha beta gamma are the interaction angles or angle between the edges the unit cell can also be defined in a little bit more quantitative manner.

(Refer Slide Time: 20:38)

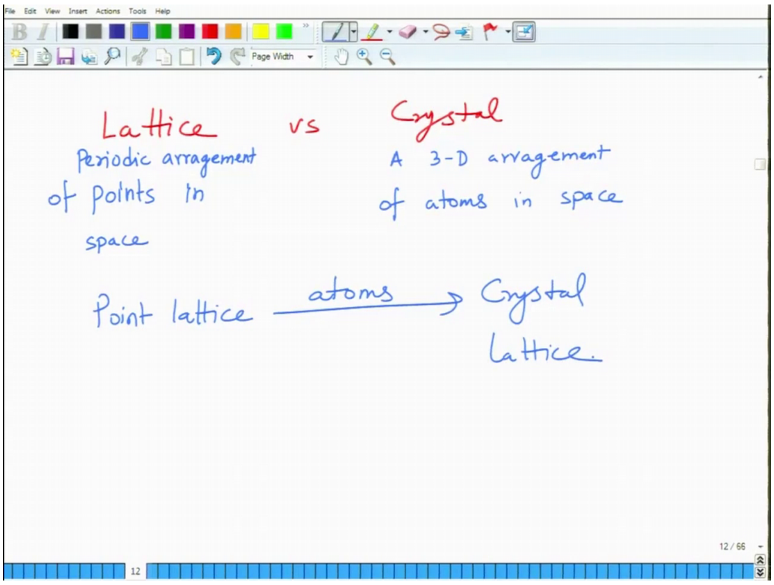


So, if you have a arrangement of points like this in space you have to define first origin ok.

Let us say this; the origin o and then the here you can choose a lattice factor R and this R can be defined as n1 a1 plus n2 a2 plus n3 a3 in the 3D or here you can just in 2D you can take. So, if you have a lattice factor let us say R this is R. So, now, you have these 2 vectors you can define.

So, these 2 vectors will make the unit cell, alternatively you could have chosen your vector as this another vector is that. So, this will be the periodic vector which will construct the lattice. So, depending up on the choice of lattice vector you can create these arbitrary unit cells ok, you can have this 1 as well. So, there are various choices by which you can make the where these unit cells, but as we discussed as we just talked about earlier it is the symmetry of that unit cell which will determined which has to be taken as a equilibrium unit itself. So, now, what is the difference between the lattice and crystal?

(Refer Slide Time: 22:32)



Can you tell me; what is the difference between lattice and crystal.

Student: (Refer Time: 22:41).

Ok.

Student: (Refer Time: 22:43).

Ok.

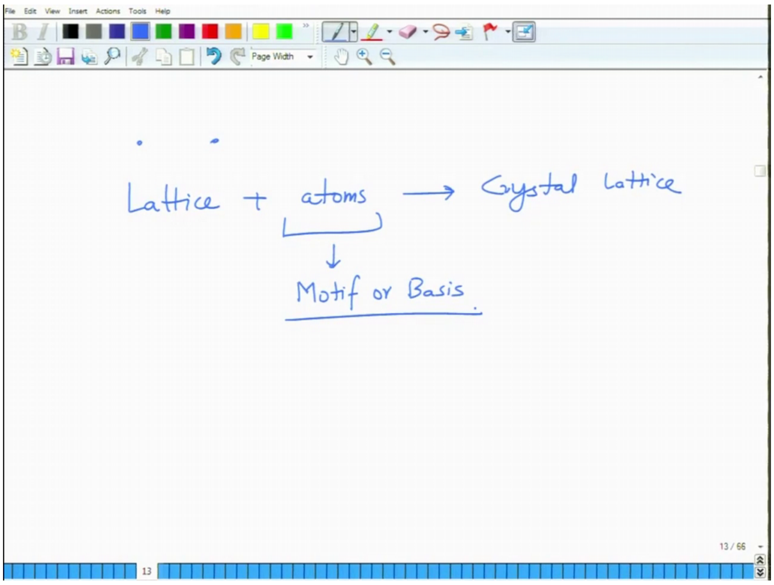
Student: (Refer Time: 22:47).

But what is the definition.

Student: (Refer Time: 22:49).

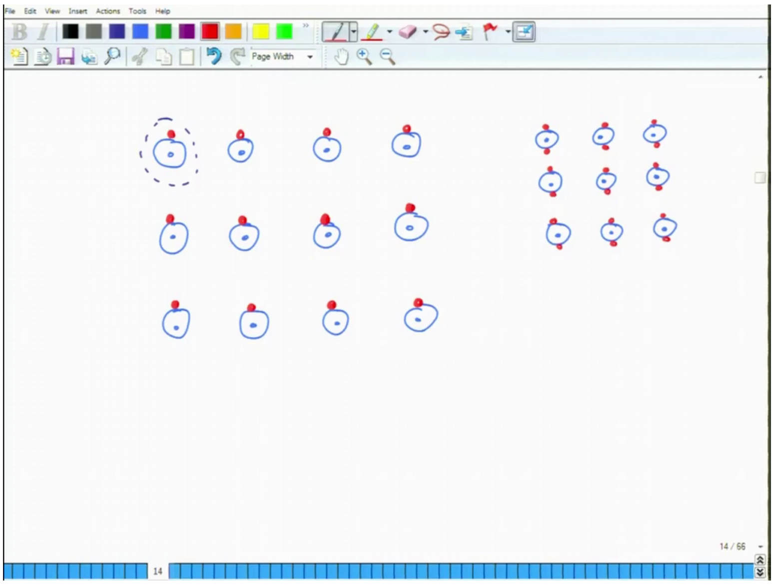
So lattice is only about the points in space or you can say periodic arrangement of points in space this is lattice and what is the crystal a 3D arrangement of atoms in a space [FL]. So, basically you can say you start with the point lattice and when you put atoms here it becomes a crystal lattice all right. So, based on this particular aspect of lattice now within this lattice if I go back to previous 1. So, I have a I have unit cell like this now if these are all atoms this will be called as a crystal lattice ok.

(Refer Slide Time: 24:20)



Now, so, we said that Lattice plus atoms make a crystal lattice and this atoms basically can be put in a more a specific term which is called as a motive or basis; some kind of object basically it could be atom it could be a group of atom, it could be a random multiple types of atoms arranges various places. So, for example, let me just again I draw a simple lattice.

(Refer Slide Time: 25:00)



There are lot of drawings here ok.

Now, what it can mean is I can just put a simple 1 atom this is the simplest form, this is the simplest 2D lattice; I can make some change here I can make this as a molecule let us say it is a it is not just 1 atom which goes to a point it is this molecule which goes to a point. So, you have replaced the points with these molecules does this make a lattice, does it still retain the definition of lattice in the previous case I did in the previous case I did now that you have a atom which is that you can consider this molecule as asymmetric atom ok; it is a group of atoms right you have a group of atom which is like this.

So, the question is does this modified motive retain the definition of lattice, let me give you another scenario instead of having this. So, I will draw it again little smaller now again I draw these atoms, now instead of putting them in this fashion I let us say I will put them in this fashion. So, these atomic arrangements now they have mod they have modified from the previous 1. So, the question raises rather they still maintain the validity of lattice they seem as if they are periodically arranged in the lattice, they are regularly spaced that sort of problem they look like as if they are following certain pattern.

But the question is do they maintain the validity of definition of lattice. So, we will discuss these aspects related to placing different kind of objects or motives in a space and how do they alter the definition of lattice and then invoke the symmetry to understand this in the next few lectures.