An Introduction to Materials: Nature and Properties (Part 1: Structure of Materials)

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Lecture – 09

Symmetry and Correlations with the Bravais Lattices

So let us now start a new lecture which is lecture number 9 on symmetry and correlations their correlation with the Bravais lattices. So, before we get into it we just want to recap what we did in lecture 8 and 9; 7 and 8.

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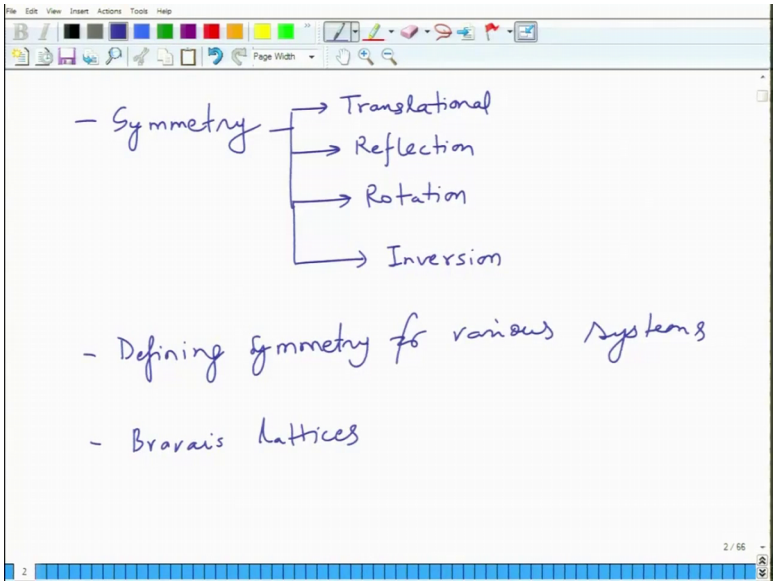

So, what we learnt there was this concept of symmetry and symmetry is not something which is just my just on the basis of look, it is on the basis of certain well defined criteria and we defined that there are 4 kinds of symmetry elements, first is translational and translational is a given for every system. So, translational is something which is generally not talked about when we define the class when we when we do the classification of crystal we do not talk about translational symmetry because translational symmetry has translational symmetry has to be there for a crystal for a for a periodic system. So, a translational symmetry, then we have reflection symmetry then we had rotation and then we had inversion ok. So, these 4 symmetry operations basically

complete. There are some other symmetry operations which are glide and screw, but these are the 4 major symmetry operations which have to be which define the crystal systems and Bravais lattices and then there are finer distinctions between the same class or Bravais lattices there are different materials with different motifs and different symmetry elements come into picture, but these are 4 basic symmetry operations which define your Bravais lattices and crystal systems.

And we also saw that wise; what is the defining symmetry for defining symmetry for various crystal systems.

Now, that is mostly governed by rotation. So, for example, for cubic system you need to have 4-3 folds, for tetragonal you need to have 1-4 fold, for orthorhombic we need to have 4-2 folds and so, on and so, forth. So, we had defining symmetry for 7 classes of crystal systems and then we looked on to Bravais lattices what is the what is the correlation of these Bravais lattices with the with the symmetry? So, for example, we were looking at 4 so, we looked at 7 crystal systems we defined them in categories of P I F C and we saw that in case of cubic you only have primitive, body centered and face centered, in case of tetragonal you had only primitive and body centered, in case of orthorhombic you had only you had all 4 of them and so, on and so, forth. So, the question was why are some of these missing?

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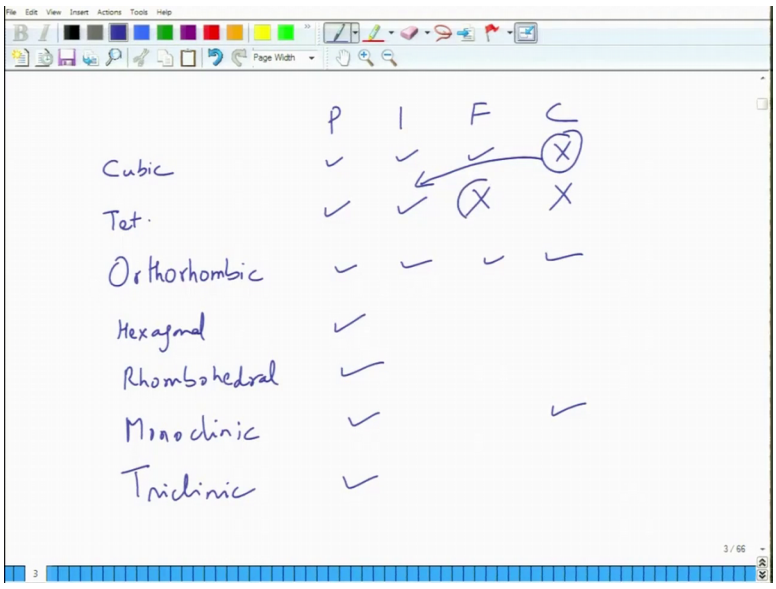

So, for example, why is cubic missing a C centred cubic missing? Why is face centered tetragonal missing? Why is C centred tetragonal missing? And so on and so forth and then of course, you had hexagonal which again had only primitive system, rhombohedral also had only primitive and then monoclinic again had only primitive and then triclinic sorry monoclinic also had C centered, triclinic had only primitive.

So, we looked at the reason of for example, C centred cubic why C centered cubic is not there the reason is because C centred cubic can be defined as body centered tetragonal and C centred cubic does not fulfil the criteria of 4-3 folds which must be present in a cube. So, although it may look like a cube it is not a cube it has a smaller unit cell in terms of polycentric tetragonal and it fulfils symmetry criteria of tetragonal unit cells. So, C centered becomes body centered tetragonal.

Similarly, now the question arises is why is that you do not have a face centered tetragonal? So, we will not go into all of them, but I will give you some examples as to why some of them are not present. So, let us say a face centered tetragonal here. So, let me just draw a unit cell here tetragonal unit cell.

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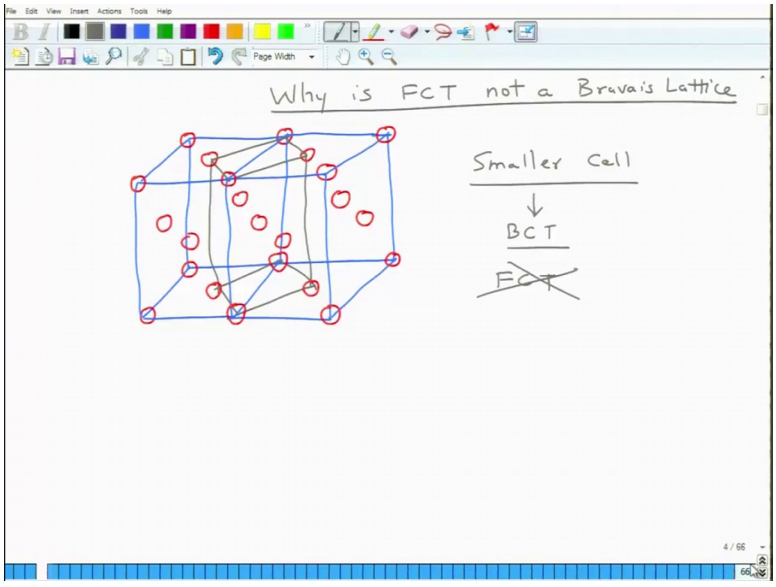

So, we will draw 2 unit cells, you might have guessed by now that they are not there because either they do not make a valid lattice or they convert into something else which has either higher symmetry or smaller ship size ok. So, this is does not look like the 2 are slightly different in sizes, but nevertheless. So, let us put the atoms here, these are 2

tetragonal cells adjacent ones let me just draw this as well and this is what ok. So, we are saying that why is face centered tetragonal not there so, we draw atoms at the centre of the faces alright, now.

So, we have drawn this here you can see that you can construct a smaller tetragonal cell in this fashion which is actually a body centered tetragonal. So, it has it has same tetragonal symmetry, but a smaller cell. So, basically we prefer a smaller cell, if you remember I earlier told you there are 2 criteria one is a smaller size, second is a symmetry. So, in case of cube cube you saw it does not follow the symmetry right. In in this case we can see that there is a smaller cell size which is preferred and as a result it it it converts it is defined as body centered tetragonal, that is why face centered tetragonal is not present in the Bravais lattices because it can always be represented by a smaller body centered tetragonal unit cell and you choose a smaller unit cell as per the criteria. So, this is why FCT is not there why is FCT not a Bravais lattice so, this is the answer for that.

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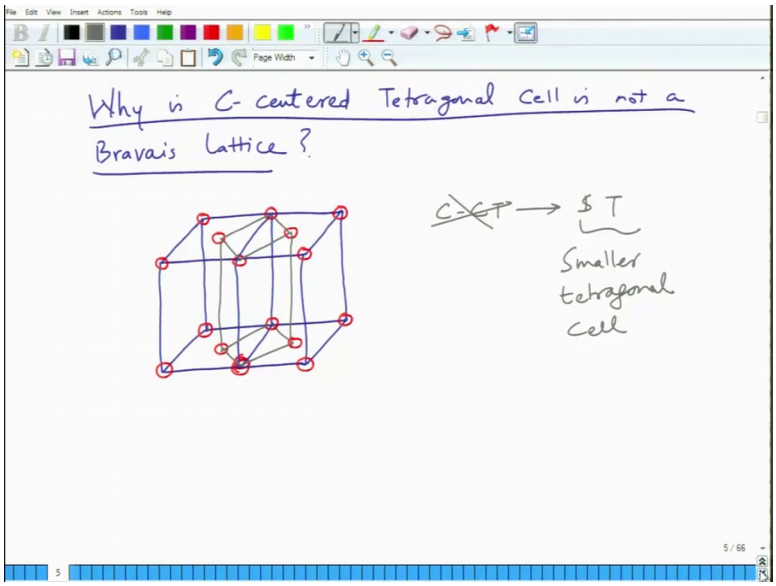

Now, you can also choose similarly you can have so, in the in the in that table now if you can go back to the table you can say that this F is nothing, but I similarly now you can see why do not we have; why is C centered tetragonal cell is not a is not a Bravais lattice. So, you can see that it is not a Bravais lattice because if I make a C centered tetragon again I will have to make 2 unit cells. Now if I put the atoms here 1, 2, 3, 4, 5, 7. So,

these are the atoms, I have put and C centered would mean that I can put an atom here, I can put an atom here, the atom here ok. So, can you tell me the answer? Because, you can always make a simple can always make a simple tetragonal cell with the same symmetry. So, the answer is C C C centered tetragonal is nothing, but simple tetragonal so, that is why this does not exist. So, basically a smaller tetragonal cell so, you can you can do the same exercise for example, for hexagonal system you do not have for hexagon.

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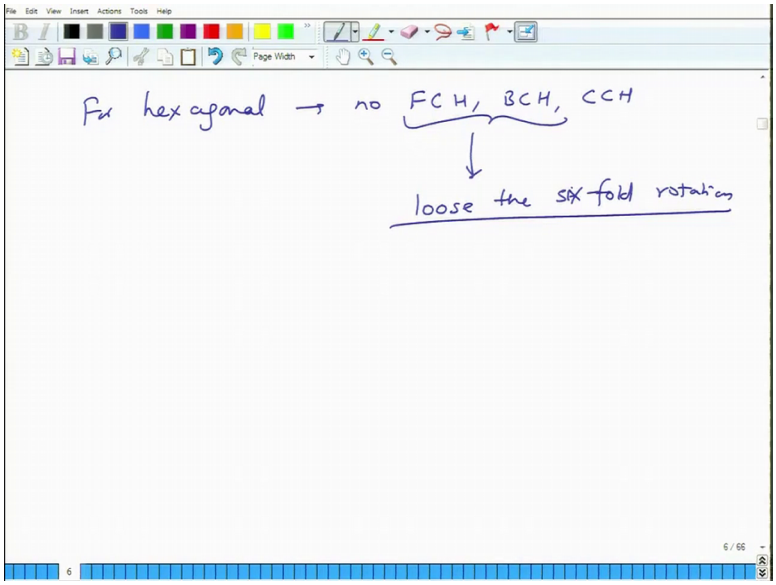

For hexagonal you can see there is no FCH, BCH or CCH the reason for that is the moment you put body centered and face centered, you lose the 6 fold rotation symmetry, it no longer remains as a hexagonal so, that is so, you can you can check it out yourself try putting atom at the centre of the unit cell and hexagonal and try to operate that 6 fold you will see that you will lost at 6 fold. Similarly you try to do that in face centered tetragonal c centred tetragonal you can see that you will lose the 6 fold symmetry.

So, now the question one more question that you can ask me is; what is the reason.

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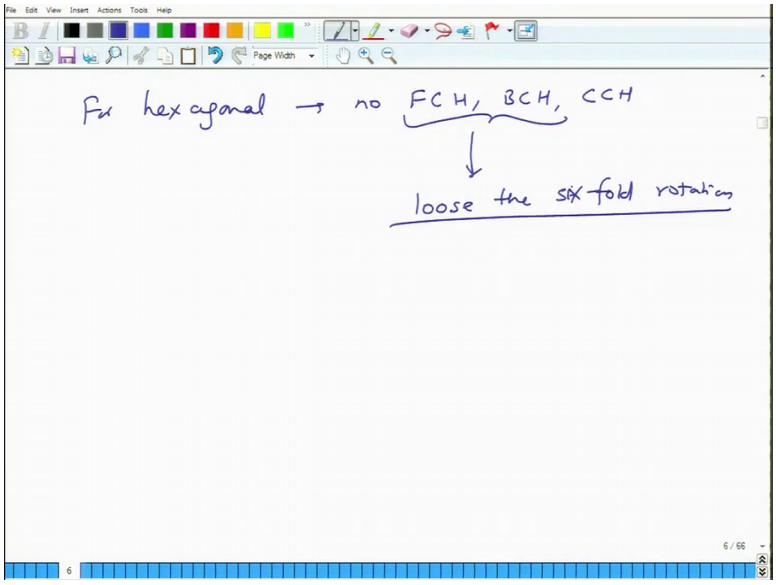

For choosing for example, in cubic FCC or BCC unit cell over their primitive counterparts you have seen yesterday that 1 FCC is made of 4 primitive lattices, what is the shape of that lattice? It is a parallelo parallelepiped right it is not a regular shape cube shape or something like that. So, the reason why you choose FCC over the primitive counterpart is because FCC has higher symmetry in cube you can make it it has higher symmetry elements, it has 4-3 folds, 2 folds and 4 folds whereas, if you choose only the primitive ones you will lose some of the symmetry elements. So, that is why FCC although it is a bigger unit cell than the primitive unit cell. So, higher symmetry despite despite larger size same is true of BCC, same is true of any other non primitive structure which is chosen in comparison to primitive structure. Now, another last thing that I want to tell you is that you can see.

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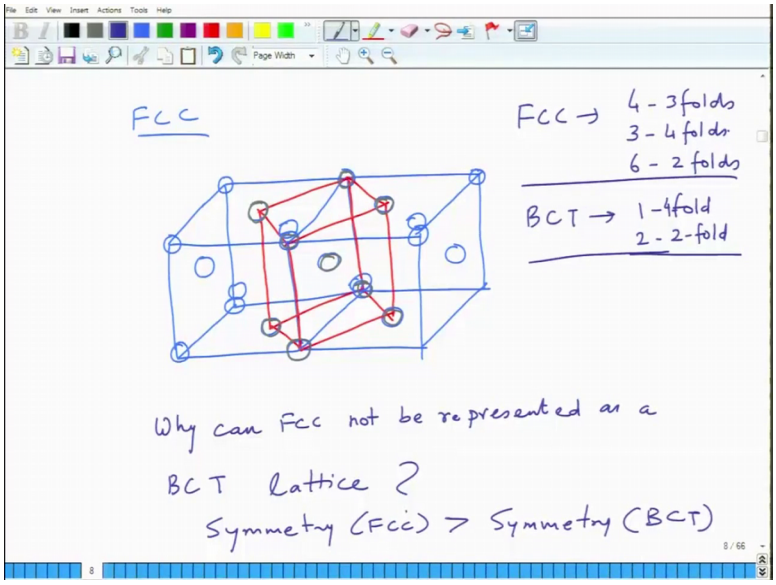

You can you have a FCC unit cell, if you draw a FCC unit cell it will look like this the question that I want to ask you is that can this FCC be represented as body centered tetragonal for example, if I draw a neighbour to it this is a neighbour right let me now colour this thing ok. So, for the sake of representation I can draw this atom as different this is body centered tetragonal.

So, question is why can FCC not be represented as a BCT lattice not unit cell as a lattice? So, you can see now you need to see the symmetry FCC has 4-3 folds, it has it has 4 folds. So, 3-4 folds and it has 6 faces so, 3-4 folds and it has 6-2 folds. In case of tetragonal you have 1-4 fold and 2-2 fold. So, although BCT has a smaller size than FCC unit cell the symmetry of FCC is higher. So, since the symmetry of FCC is higher we choose a higher symmetry.

So, when you have this conflict of symmetry then symmetry prevails when the symmetry is similar, then you choose the smaller size ok. So, these are the 2 defining criteria's one is size.

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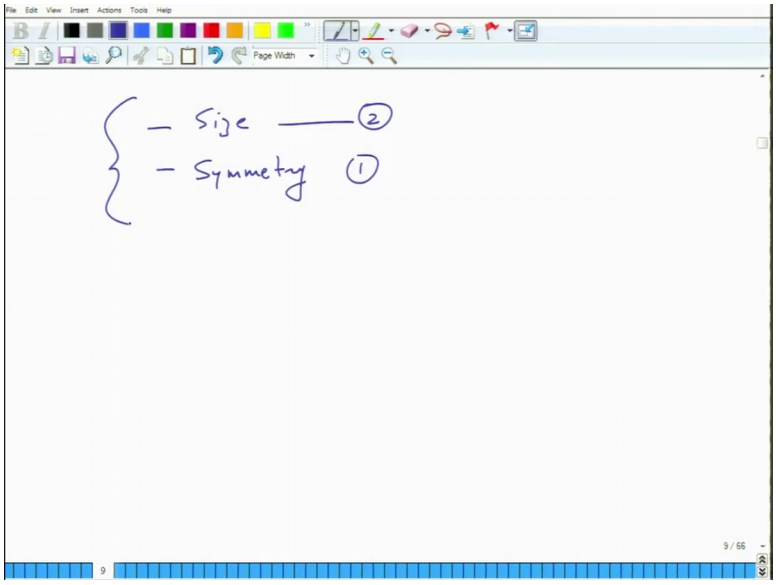

Second is symmetry and symmetry prevails over the size so, this is the first criteria and then this is the second criteria. So, now, you can see we have seen why do not we have 28 Bravais lattices why do have only 14 Bravais lattices and the reason lies in symmetry that some of them some of them can be represented either by higher symmetry structures or by smaller size unit cells or in some cases they do not represent the symmetry of the crystal system at all for example, in the hexagonal system if you try to draw C centered or F centered or I centered unit cells you tend to lose the symmetry defining symmetry of the crystal system itself.

So, these are certain considerations that we take into account when we talk about the crystal systems and symmetry. So, I hope now there is some clarity on why is there a why do you have 7 crystal systems which are defined on the basis of symmetry each of these has a defining symmetry and it is the combination of symmetry operations which defines in which class a particular shape will belong to and the choice also as we said in the beginning you have multiple choices of unit cells, you still choose smaller unit cell, you used to choose a unit cell which is highly symmetric. So, so in the primitive cell so, now it is clear.

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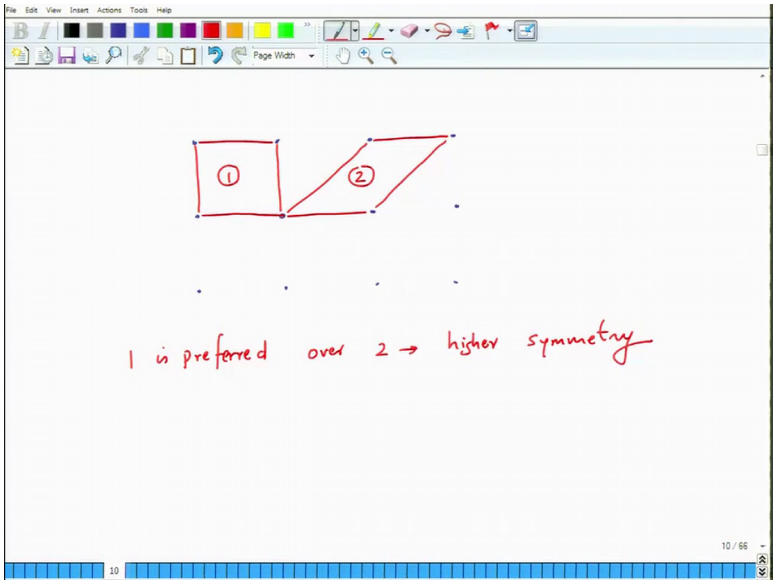

So, if you look at this for example, as an example this 1D, 2D lattice. So, here you can see now that we choose we choose this unit cell in preference to either this so, 1 this is 2. So, 1 is preferred over 2 because of higher symmetry and this is nothing, but the combination of so, here rotational symmetry plays an important role. So, that is one very important symmetry is translation we do not do not talk about because if a lattice is there it has to have a translational symmetry if it does not have translation symmetry the whole chapter is closed we do not talk about symmetry at all.

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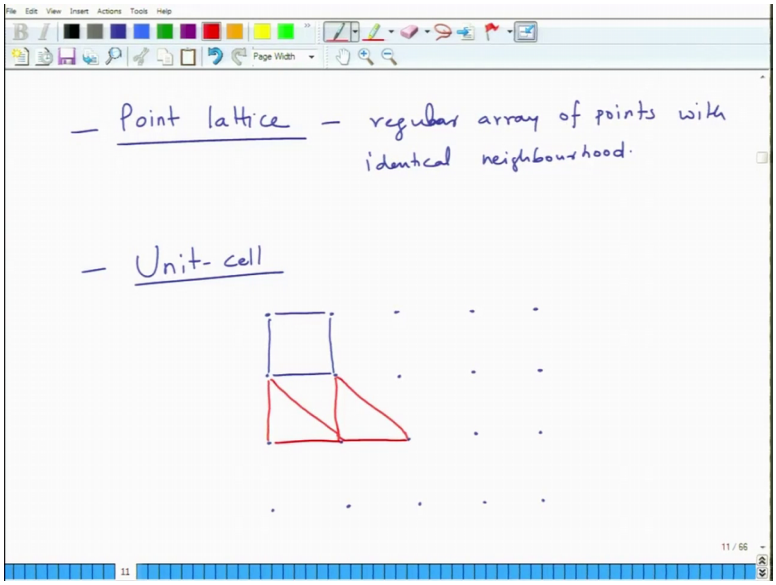

So, let me now summarize the whole crystallography in a few minutes so, what we did was we started with we started with point lattice point lattice is nothing, but regular array

of points in a space with each point having identical neighbourhood. So, regular array of points with identical neighbourhood, then we defined within the point lattice you can you need to have you can define a unit cell right, unit cell is defined as the smallest repeatable unit which can be translated into the lattice without creating any gaps ok. So, for example, this is now which is this as a unit cell or we choose some other shape as a unit cell, but we do not choose for example, this as a unit cell all right if you choose this as a unit cell then this would be the repeating unit.

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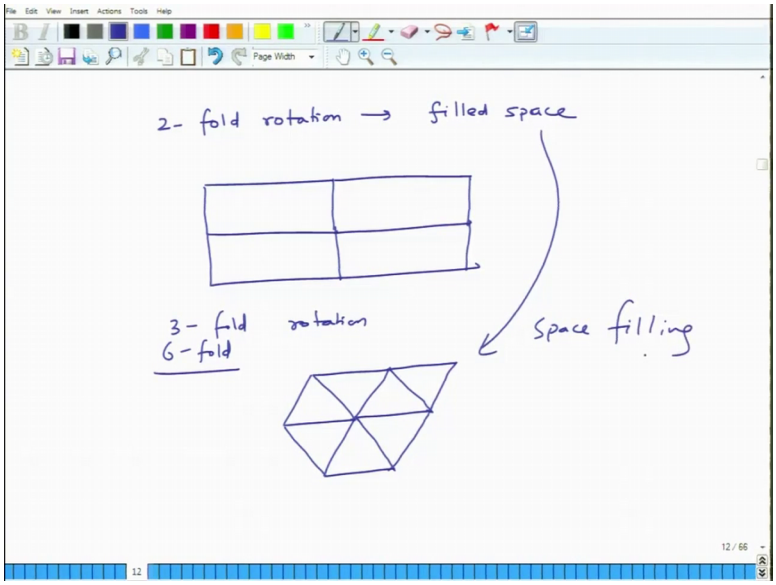

So, you will leave these gaps in between so, there should be no gap at all so, that is why if you look at the rotation symmetry there are certain operations which are so, you can see that twofold rotation you have filled space right . So, if you have rectangles lined together these are rectangles have 2 fold symmetry is right this is a rectangle. So, all these rectangles will fill the space there are no empty spaces. 3 fold rotation again you will fill the spaces now of course, this will make a hexagonal symmetry, but you can see in the case of cube for example, right. So, all these will fill the space is 3 fold and 6 fold right again space filling. So, space filling is important criteria if you look at 4 fold the rectangle.

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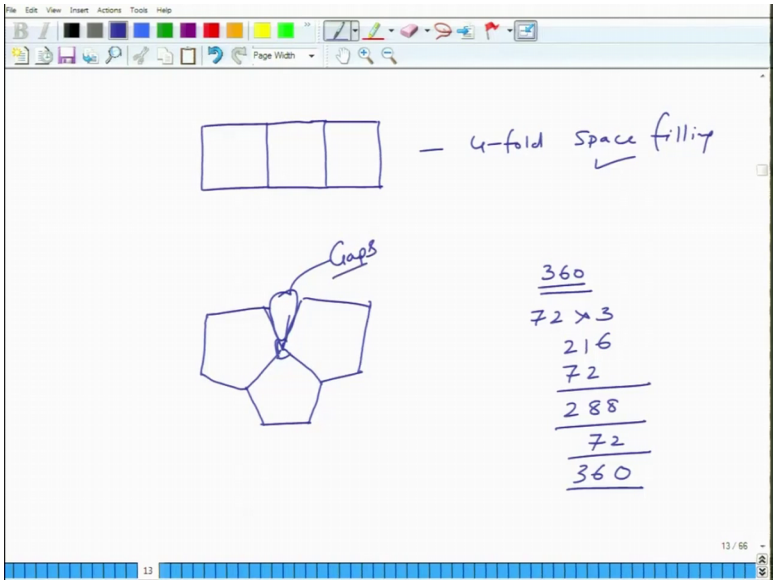

The squares all of them will fill that space. So, when we talk about threefold you talk in the context of for example, cube 3 fold you cannot talk in cubic because triangles do not fill their space in a regular fashion triangular lattice because one lattice is upside down second is upside up. So, as a result you do not talk about the triangular lattice um. So, these will fill that space 4 fold will fill the space filling.

However when you look at the pentagon now we look at the pentagon you try making a pentagon now in bit around it. So, you will see that if you try making a pentagon like this you will see if you create pentagons regular pentagons would not be able to fill the. So, you will have some gaps. Now these angles of course, around angle around a point you need to have 360 degree completed and since each of these angle is how much? This is 72 this is 72 another pentagon will give you 72. So, it does not make a multiple of so, 360 72 into 3 will give you 216, if you add another 72 to it will give you 288. So, if you add another 72 it to it will give you 360, but you cannot have 5 pen 5 pentagon sitting around a corner. So, if you try building now this is one if you try building around it this will go something like that. So, you leave a gap here similarly if you try to do the same exercise on other points you will try leaving gaps. So, pentagons do not fill the space. So, there are gaps so, there are gaps in the structure with pentagon filling.

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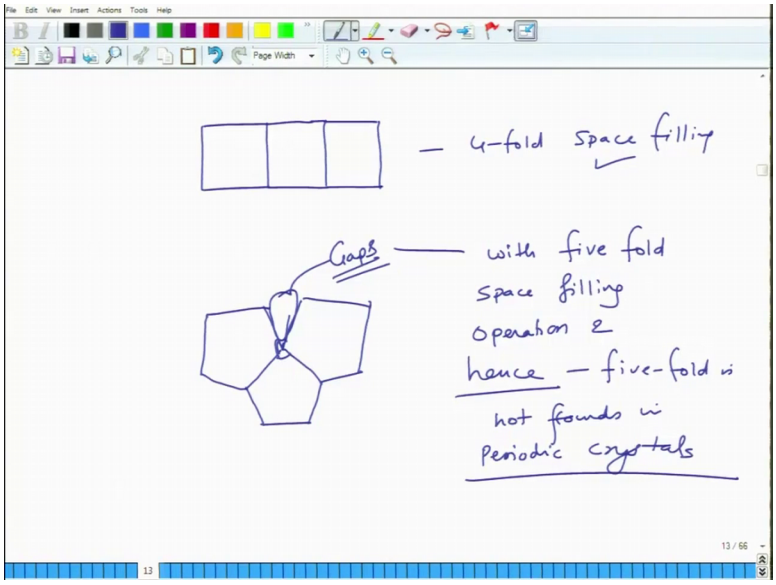

And hence 5 fold is not found in crystals in periodic crystals because there is no space filling you leave gaps in the structures ok. So, this was another thing which has to do with the and then we looked at lattice parameter the concept of lattice parameters which is a, b, c, alpha, beta, gamma and correlations between these will are dependent upon the crystal systems and Bravais lattices.

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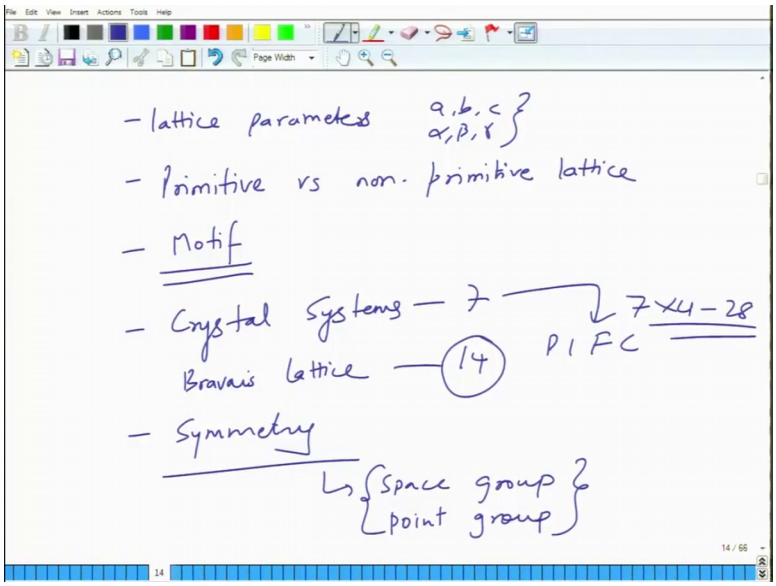

Then we looked at what is primitive and verses non primitive lattice and then we looked at what is the concept of motif this is a very important thing motif or basis because motif of bases will eventually determine how bigger unit cell be, what kind of symmetry will it follow and we have not seen about it, but what kind of space and point group will it

have. So, this is a very important concept and then we moved on to the concept of crystal systems and Bravais lattices.

So, you have 7 crystal systems you have 14 Bravais lattices we have seen why do not we have 24 there are possibilities are P I F C. So, if you multiply 7 into 4 it should give you 28, but we have only 14 and the reasons lie in symmetry. So, we saw the symmetry operations and we saw that depending upon the defining symmetry of the crystal system you choose a unit cell which is either smaller in size it has higher symmetry and based on those considerations we come up with only 14 Bravais lattices, we do not have 28 Bravais lattices.

So, this is sort of a short primer on crystal systems, Bravais lattices, symmetry and in total on crystallography as to how atoms are arranged in a in a crystal and why are there 8 in this in such a fashion, how can you classify them in different classes. There is something which leads further from this is a space group endpoint group ah, but we will not consider that in this class it is beyond the scope of this, but if somebody is interested he can he or she can look at the books which can give you more information on. So, on space and point groups so, any elementary book on.

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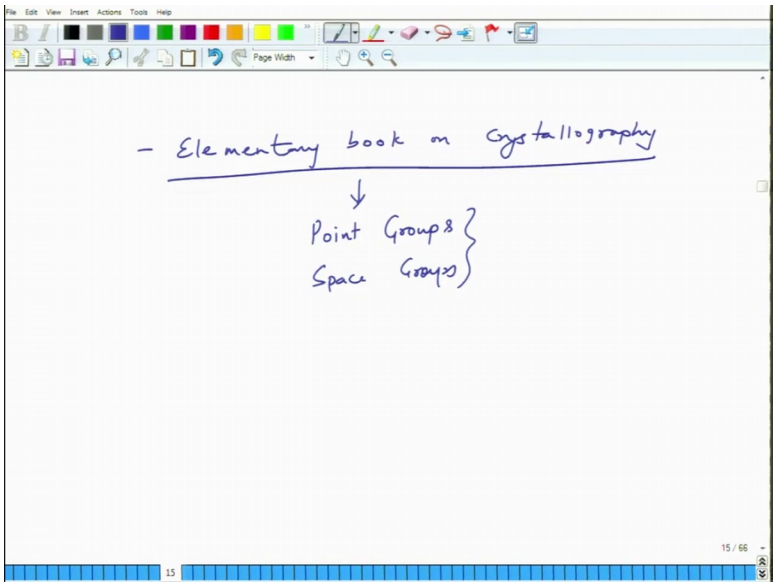

Book on Crystallography will give you knowledge of point groups and space groups. So, point group and space groups are basically further classifications of crystals. So, within one crystal class, let us say within the cubic crystal class you will have various other

connotations depending upon how atoms and molecules I mean most of these are not single atoms ok, most of the compound most of the materials are compounds. So, in compounds how motif arranges itself at various sites will determine the will be determined by will determine their arrangement and this will be this will give rise to us they can be classified on the basis of point in space groups.

So, we will leave this out of discussion for this class we will now move on to next topic which is on miller indices which is a way to classify crystals and understand their various properties.