Structure of Materials

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Lecture - 10
Chapter-02
Geometry of Crystals: Symmetry, Lattices

The next crystal, we make is using the body centered cubic Lattice. So, we take the body centered cubic Lattice.

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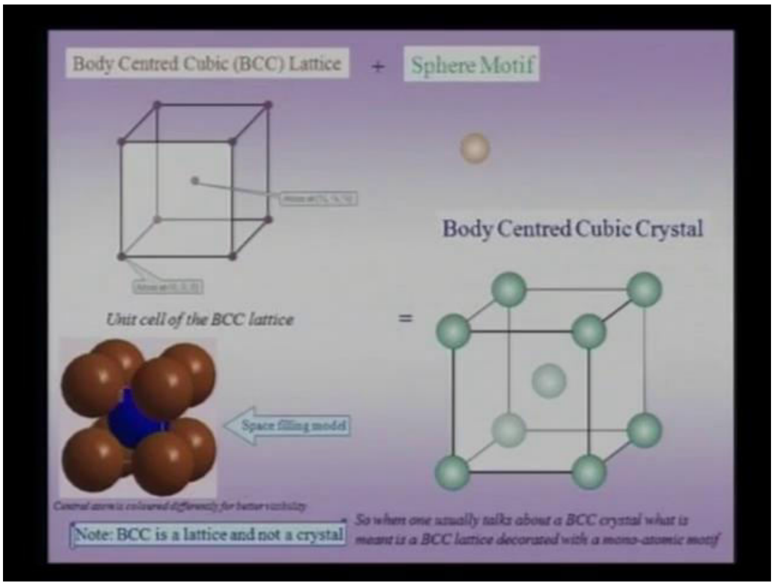

Body Centred Cubic (BCC) Lattice + Sphere Motif

Unit cell of the BCC lattice

= Body Centred Cubic Crystal

Space filling model

Central atom is coloured differently for better visibility

Note: BCC is a lattice and not a crystal

So when one usually talks about a BCC crystal what is meant is a BCC lattice decorated with a mono-atomic motif

Where in we have an lattice position at 0 0 0 and a lattice position at half, half, half and I put a very simple spherical motif on this lattice. The crystal I obtain is called a Body Centered Cubic Crystal. So, often casually, there is a term used in literature a B C C Crystal. So, we have to remember B C C is a lattice and the crystal typically, when I say a B C C crystal what they mean is a simple spherical motif which is going on to decorate the B C C lattice. If I have a more complicated motif which goes on to decorate the B C C lattice then I do not use a phrase B C C Crystal in usual sense.

So, this is an important point to note, that for an instance when I use the word simple cubic it refers to a lattice and similarly, when I use the word Body Centered Cubic it refers to the lattice and when I am mono atomically or for the instance single sphere to decorate the lattice I get a Body Centered Cubic Crystal. So, the crystal in the ballanstic view a shown on the right hand side where in these spheres are all sitting in the corners of the cube plus the body centering position.

Now, there is a space filling model also shown here, which is also showing the same crystal the B C C Crystal or I say just said the B C C lattice decorated with the single sphere motif, in some of these figures we will shed the spherical entities in different colors it should be obvious that all these entities are identical and the shading in these contexts have been done merely for better visibility. So, the blue sphere is no different from the red sphere and the shading has just been done.

So, that you can see or the see the body centering position the or the sphere sitting in the body centering position a little more clearly. We will come across later on various other types of crystals where in the central atom could be different from atom sitting in the corner, in such cases of course, we have to be clear that they are actually different atoms, in this case this is merely for better visibility. So, let me show you a physical model of the B C C Crystal. So, this is my bollenstic view of the B C C crystal.

So, in this case I have to assume that these spheres are atoms and the unit cell adjusts are marked in red and these are additionally just it functions to these other strands perform two functions, one they hold the centre atomic position, but additionally they also show the connectivity, in other words in a B C C Crystal the atoms are touching along the body diagonal. So, this atom is located in the centre touching the atom which is located at the corner.

On the other hand the atom sitting in this corner is not touching the other atom which is sitting in the corner. So, we have to remember that, so the connectivity is between the atom sitting in the corner and the atom sitting in the centre, but not along this direction. On the other hand unit cell edge is along these directions. So, this is a bollenstick model of the B C C Crystal and we have to notice that, this crystal has got the complete symmetry of the lattice it has got a 4 by m 2 bar 3 by m symmetry which I will write down on the board.

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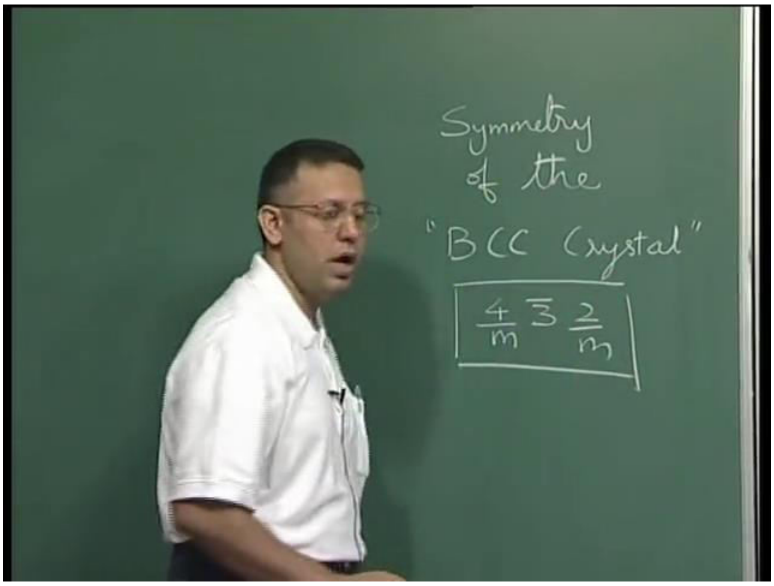

And I am using the phrase B C C Crystal in the exact sense which I just described to you. And this also happens to be the symmetry of the lattice from which I started off, let us also look at the other view of the B C C Crystal and in this case I will have to look at a space filling model which is on the left hand side of the figure.

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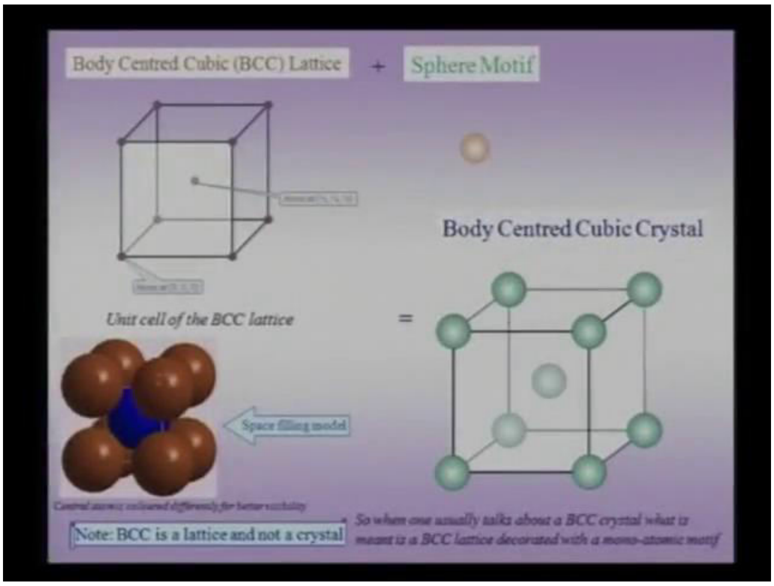

Body Centred Cubic (BCC) Lattice + Sphere Motif

Unit cell of the BCC lattice = Body Centred Cubic Crystal

Space filling model

Central atoms coloured differently for better visibility

Note: BCC is a lattice and not a crystal

So when one usually talks about a BCC crystal what is meant is a BCC lattice decorated with a mono-atomic motif

So, this is a space filling model and when we want to understand a crystal will have to look at all these alternate views. So, that I can understand the crystal in totality. So, once again we have to remember in a B C C Crystal the atoms in the corners do not touch the other atoms in the corners of the or the vertices of the cube, it is a touching is along the central atom which is being shaded in blue is touching all the other 8 atoms which are sitting on the corners of the unit cell.

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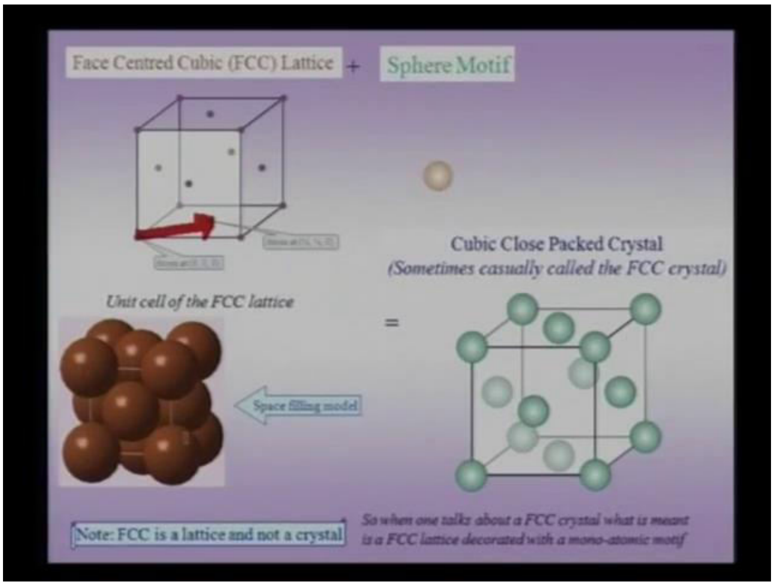

Face Centred Cubic (FCC) Lattice + Sphere Motif

Unit cell of the FCC lattice

Space filling model

=

Cubic Close Packed Crystal
(Sometimes casually called the FCC crystal)

Note: FCC is a lattice and not a crystal

So when one talks about a FCC crystal what is meant is a FCC lattice decorated with a mono-atomic motif

The next crystal we consider, is made out of the face centered cubic lattice and as before I mentioned Face Centered Cubic when I say in isolation the word face the acronym F C C it refers to a lattice and not to the crystal. And whenever, I say use the word F C C Crystal what I typically mean like in the case of the B C C is that a single sphere motif has gone on to decorate the F C C lattice.

And the crystal I get will be actually, something known as the cubic close pack crystal, we will look at this crystal in a lot more detail in coming topics later on, but for now, we have to remember that we sometime call this F C C Crystal, but more technically this is a cubic close pack crystal and it has been obtained by, starting of an F C C lattice and putting a sphere motif or an atom single atom motif or a single ion motif on each lattice point. So, in this case, we have already seen the shortest lattice translation vector is from the 0 0 0 position to the half half 0 position. So, I can draw my shortest lattice translation vector between these 2 points.

And this is my shortest lattice translation vector. We are, as when we were dealing with this lattices we have made it absolutely clear that every lattice point is identical and just because, unit cell has been drawn with the origin here, this looks at the centre of the face, but I could have also chosen the this as the origin and drawn the lattice and the lattice would be no different or the unit cell would be no different.

So, this is the F C C Crystal, as we call in normal language and we have got a space filling model of the F C C Crystal. In this case we have to notice that, the atoms are touching along this direction, the face diagonal direction and not along any other direction. So, we see the space diagonal directions and there is another face diagonal direction. So, let me go and pick up a model to show you this F C C Crystal.

So, I got here with me, a unit cell of the F C C Crystal where in these blue spheres are atoms, these are cells of the edge as marked in red. And these additional strands are the directions of connectivity which also serve the original purpose of holding the central sphere in space. So, the atoms are touching along this direction, and as we shall we shall see later this direction in allocated to miller indices will be labeled as 1 1 0 that kind of directions. So, we can see that there is considerable amount of space in the centre, the centre of the body and this aspect we will consider little more detail later.

So, this is my F C C Crystal and we will see there are important directions in this F C C Crystal which is the body diagonal direction which we have placed upward, now or if I want to show along this direction the body diagonal direction is a important direction in this F C C Crystal and we will take up, aspect very soon. Now, we reduced a phrase that this is also called a cubic close pack crystal and this is because, it is made up of closed pack planes. The highest density I can obtain in 2 dimensions is by, considering an hexagonal layer like this.

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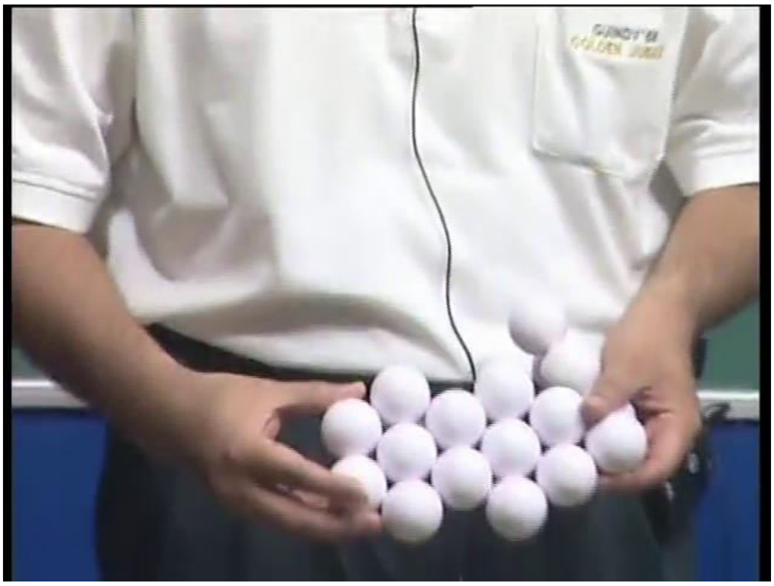

This is my hexagonal plane of course; this plane can be grown to an infinite plane by putting many more spheres. So, this is my infinite 2 dimensional close pack structures. So, in 2 dimensions this is the close packing I can get and from here, I can go on to make a crystal like that which is a cubic close pack crystal starting with planes like this, and this operation we will do little later.

So, in 2 dimension this is my close pack structure in 3 dimensions, one of the possible close pack structures is this structure which is the face centered cubic crystal which is nothing, but an F C C lattice decorated with a single sphere. So, let me look at the unit cell of the same F C C Crystal, but now in the space filling model. So, this is my space filling model of the F C C Crystal. And you can see very clearly the atoms are touching along these directions.

And also that the atoms are not touching along the cell edges. So, this is my cell edge, and this is my another cell edge. So, the atoms are not touching along the cell edge, but they are touching along these directions. So, this is my space filling model of the F C C Crystal, we will come back to these kind of space filling models and their importance is specially in understanding various concepts related to the F C C Crystal in a later topic.

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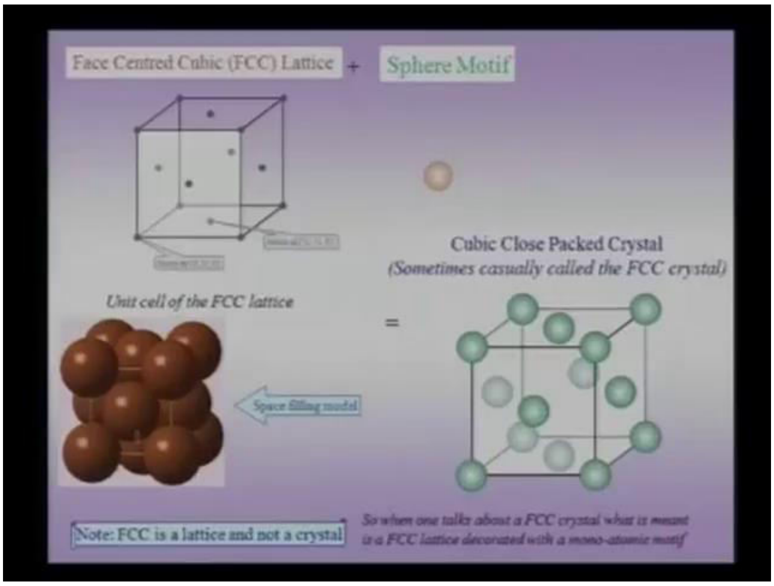

Face Centred Cubic (FCC) Lattice + Sphere Motif

Unit cell of the FCC lattice

Space filling model

=

Cubic Close Packed Crystal
(Sometimes casually called the FCC crystal)

Note: FCC is a lattice and not a crystal

So when one talks about a FCC crystal what is meant is a FCC lattice decorated with a mono-atomic motif

So, just to emphasize again whenever, I loosely use the word F C C Crystal I mean a single sphere decoration of the F C C lattice and only and one and only under these circumstances is a structure I obtain will be a close pack structure, I could chose more complicated motifs to decorate the F C C lattice and in all these cases, I would not obtain a close pack structure. We will take up examples of these, but just a prelude to this taught process for instance I can use a pullery in molecule to decorate the F C C lattice to obtain an F C C crystal or a crystal which has the F C C lattice at it is underline lattice.

And such it is obvious that the F C C or the crystal obtained by putting a pullery in molecule in every lattice point is not a closed pack crystal. So, just because, when I use the word F C C I have to remember it is a lattice and merely just because, the lattice is F C C the crystal I get from decorating this lattice, need not be a close pack crystal. That is point has to be absolutely understood.

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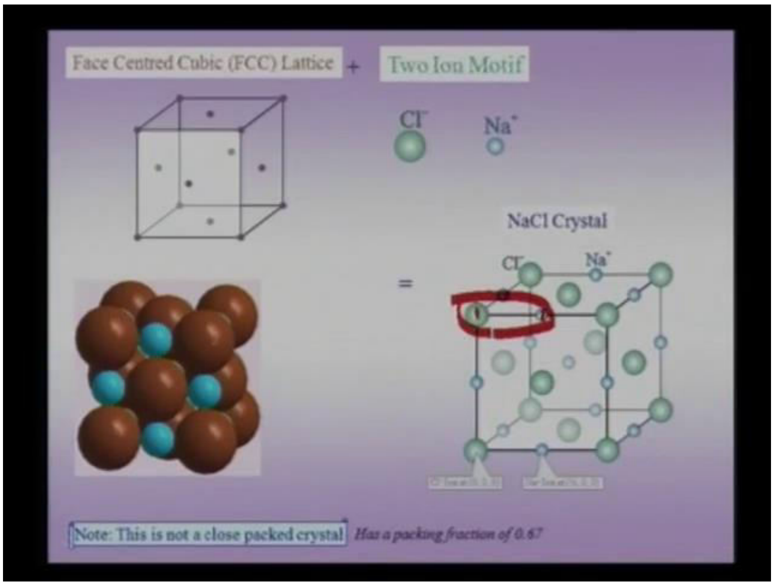

Face Centred Cubic (FCC) Lattice + Two Ion Motif

NaCl Crystal

Note: This is not a close packed crystal *Has a packing fraction of 0.67*

So, let us take up another example, which is re-enforcing the point I just now, mentioned. This is for instance a F C C lattice which has been decorated with a 2 ion motif a chlorine ion and a sodium ion. This is nothing, but the common salt structure, which is the N a C l structure and the la crystal I obtained is the one which is shown in the diagonal on the right. So, now if you see that this is diagonal you see that, all the green atoms or the green spheres are be more precise in this case green is a chlorine ion forms an F C C lattice.

Equivalently all the possessions of the sodium ions also form an F C C lattice. This is an important point, and we have already dealt in detail with the concept of a sub lattice. So, now, we can think of 2 sub lattices in this case 2 sub lattices of F C C type. So, I can have one sub lattice of F C C type with it is origin at this position, another sub lattice of the F C C type with it is origin at half 0 0 which is nothing, but the edge centre the sub lattice at the origin is occupied purely, by the chlorine ions which is the larger ion, the sub lattice at with it is origin at half 0 0 is occupied by sodium ions.

And the crystal I get can be visualized, as an interpenetration of 2 sub lattices of the F C C type. So, to go over this concept once again, I have used an F C C lattice I have used a 2 ion motif now, the motif would be; obviously, a combination of a single ion of sodium and a single ion of chlorine this is my motif. And this motif decorates every lattice point.

So, if I have this lattice point being decorated by a sodium and a chlorine. So, well this lattice point we decorated by a chlorine and a sodium.

And of course, it is left as an mental exercise to the reader actually, that if I decorate every lattice point with this kind of a motif then I would get the crystal, as shown in the figure. So, this is an exercise which everybody should do in this case perhaps somewhat simple to visualize that, how this kind of a motif goes on to decorate this lattice, but in certain other cases it may not be that obvious and a little visualization is required. So, please spend some time over this particular structure to understand, how it is made up of this lattice and the motif as shown.

And I said mention this crystal I obtained can be taught of as 2 interpenetrating F C C Crystals or what I am call is the F C C sub crystals, which are nothing, but a sub lattice of F C C decorate by chlorine, another sub lattice of F C C type decorated with sodium ions and I get 2 interpenetrating F C C Crystals or F C C sub crystals which gives me the sodium chloride structure. Now, let me look at space filling model of the same which is shown on the left hand side and you can see that, there are these ions of sodium and the ions of chlorine which is occupying this structure.

Now, energetically as we will see later, that it is not preferable that my ions of like type for instance the chlorine ions do not touch other chlorine ions, my sodium ion atoms do not touch other sodium ions and this is what is energetically preferable which is why you see that, these ions of the same type for instance the red spheres do not touch the other red spheres. So, let us look at actual models of these, so this is my bollenstic model of the sodium chloride structure in this case, we should remember that there have been additional red line in a sphere which are wrong.

In fact, the unit cell edges are only the corners of the cube. And these are seats for instance are the chlorine ion, it is the seat of the sodium ion and you can see that, in this space filling model that this ion for instance does not, does touch this ion or this ion does not touch this ion. Similarly, the sodium ions are also spaced apart while the presence of these chlorine ions and they do not touch each other. So, this structure looks very nice and you can see it is a beautiful periodic array and this is one of the first structures to be analyzed by, extra diffraction and by brag. So, this is one of the beautiful structures.

So, you should remember here, that there is actually speaking in a covalent bonding sense there is no molecule of sodium chloride that is we kept in mind there, is no molecule it is nothing, but an array of sodium and chlorine ions occupying space and we cannot identify a sodium and a chlorine molecule or any such concept which are not applicable to the crystals I am describing here. So, this is my beautiful sodium chloride structure.

And, so the difference between this kind of sodium chloride structure, which is based on the F C C lattice and a simple sphere decoration of the F C C lattice is obvious, there is no touching of ions for instance along the 1 1 1 direction. But, still the shortest lattice translation vector is the vector connecting this green sphere to the this green sphere, and this is nothing but, the half, half 0 kind of vector. Now, as I mentioned this structure, is not obtained from mono atomic or a no mono sphere decoration of the F C C lattice and this is not a closed pack structure.

The packing fraction of this kind of a structure, is 0.74 or 74 percent of space is occupied by spheres and as we shall see, this is only 67 percent. So, the packing fraction of this kind of a structure is lower and therefore, I cannot call it a closed pack crystal, merely because, it is based on the F C C lattice. So, this has a lower packing fraction which is 0.67. So, I say pointed out we can start with an F C C lattice and decorate it with more and more complicated motifs some more examples, we will consider later in the course. In the previous example, where in we started with the F C C lattice reduced to different kind of ions decorate the lattice. In this case we consider, what is known as the Diamond Cubic Crystal.

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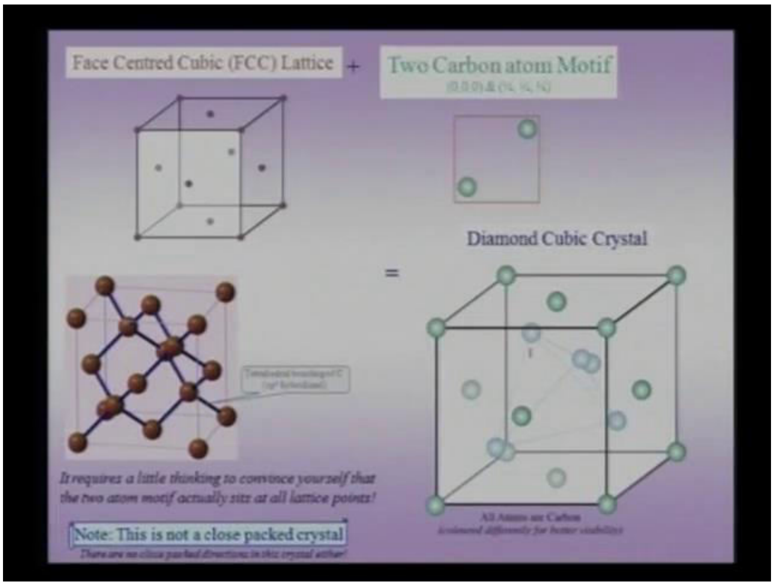

Face Centred Cubic (FCC) Lattice + Two Carbon atom Motif

(0,0,0) & (¼, ¼, ¼)

=

Diamond Cubic Crystal

It requires a little thinking to convince yourself that the two atom motif actually sits at all lattice points!

Note: This is not a close packed crystal

There are no close packed directions in this crystal either!

All Atoms are Carbon

(coloured differently for better visibility)

In the diamond cubic crystal we have atoms of the same type which is nothing, but 2 carbon atoms and as we might be knowing that the carbon atoms in the diamond are s p 3 hybridized; that means, the bond angle between, central carbon and all are tetrahedral. So, they are tetra-he rally bonded to the single carbon atom. And this tetrahedral bond pervades in 3 dimensions to complete the kind of structure I am showing. So, let us start with this F C C lattice as before.

Let me, put the 2 atom motif and in this case the 2 atoms of carbon allocated at 0 0 0 and half quarter, quarter, quarter. So, if I do that I obtain a crystal which I shown here. So, I have an atom at 0 0 0 another atom of at quarter, quarter, quarter. So, I take this 2 atom motif and I put at every lattice point of the F C C lattice at this lattice point and this lattice point, so forth and I will get this crystal. In the figure shown, which is the bollenstic kind of a model we have to remember that atoms have been colored differently, for better visibility and all atoms are nothing, but carbon.

So, this is carbon atoms and just for better visibility, we have shaded them differently. The central carbon atoms located within the unit cell, form a tetrahedron as drawn by this outline. So, this is just to make the visibility better that these form actually, a tetrahedron. And an important point which is to be noted, in this crystal is that, it has no normal 4 fold rotational symmetry. So, this in an important point to note, that the diamond cubic crystal has no rotational pure rotational 4 fold symmetry.

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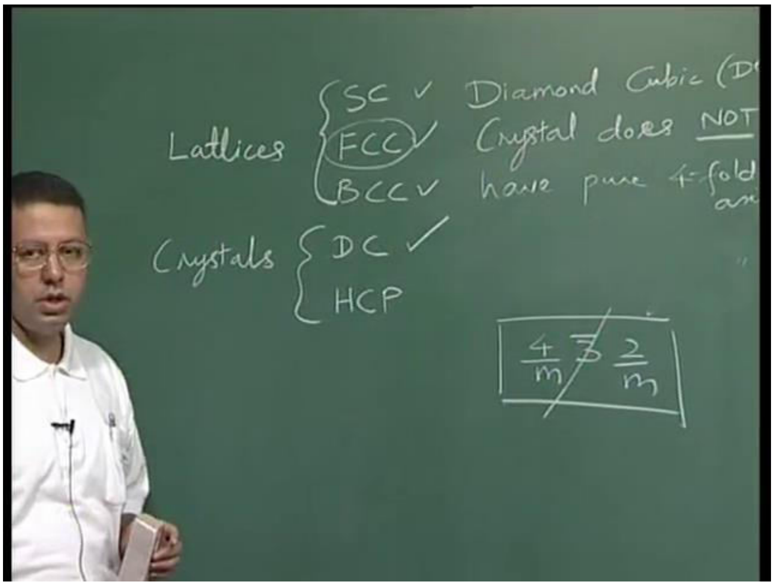

And the symmetry of the crystal has been lowered, below that of the lattice. So, this is not symmetry of the crystal any more. As, I am talking about this diamond cubic often you will find an acronym for diamond cubic as B C C, I will utilize this option to actually write down all the common acronyms which we use for instance we use the acronym S C, F C C, B C C, D C and one more acronym we will come across later is H C P please remember they look very common in terms of their description like we have to remember these 3 are lattices and these 2 are crystals.

We have already constructed crystals made out of these lattices, and additional just now, we are considering a crystal made out of this F C C lattice, but is called the Diamond Cubic Crystal. And we have seen that this Diamond Cubic Crystal does not, have a 4 fold rotation axis, a pure 4 fold rotation axis. we can analyze the symmetry of this crystal in a little more detail later on but, for now, it is important to note that the symmetry of the crystal has been lowered, with respect to that of the lattice by the presence of additional atoms in the motif.

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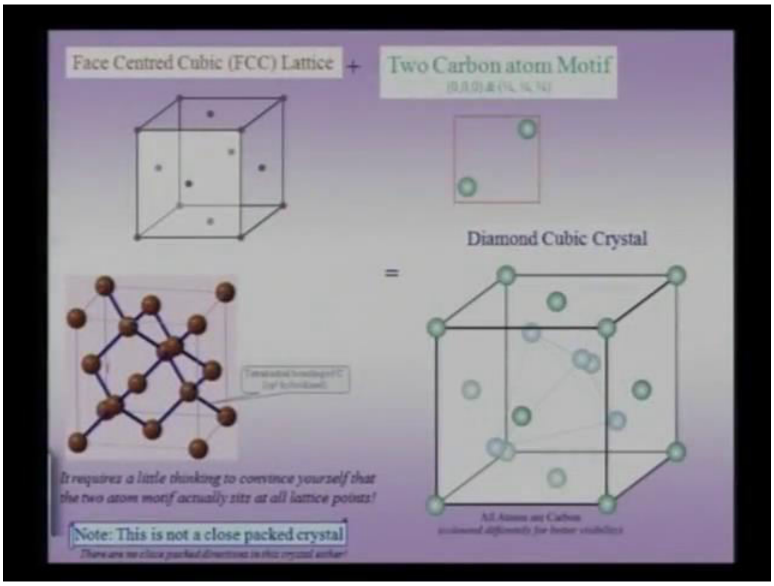

Face Centred Cubic (FCC) Lattice + Two Carbon atom Motif

= Diamond Cubic Crystal

It requires a little thinking to convince yourself that the two atom motif actually sits at all lattice points!

Note: This is not a close packed crystal

Now, this kind of a model which is shown on the left, is a important kind of model which you would have seen in text books, where in this tetrahedral order I was talking about where in the central atom,, is touching this atom and is touching this atom, then it goes this tetrahedral order pervades in 3 dimensional space to occupy the entire space. Now, again we note that, this crystal we obtained is not a closed pack crystal. Another example, to emphasize this fact that just because, some crystal is based on the F C C lattice it need not be a closed pack crystal.

May be we will perform this a later or is left as an assignment to reader to actually, calculate the packing fraction for this crystal. Now, this crystal is completely covalent and is very different from the kind of bonding, we considered in the sodium chloride crystal. So, this bonding difference also we will consider very soon and we will, try to analyze crystals on what kind of rules would the one what kind of a crystal would form, but we have to remember that this diamond cubic crystal is covalantly bonded.

But, never the less, we cannot call any small part of this crystal as a normal covalent molecule, but this entire order pervades to this entire crystal and therefore, this is a completely s p 3 hybridized atom of carbon which is give rise to this crystal structure. In this kind of a crystal as we know the, Diamond Cubic Crystal has very interesting properties for instance it is one of the hardest materials, and it has a very high refractive index, it is has a very poor thermal conductivity or we would emphasize it got very poor electrical conductivity, but has got very good thermal conductivity.

So, this is a very strange kind of a combination of properties typically, when you are talking about electrical and thermal conduction it is used to the electrons which are responsible for both. And therefore, electrical conductivity and thermal conductivity go hand in hand, in this crystal we find that has got both thermal conductivity, but very poor electrical conductivity. So, it is an insulator. So, to summarize, the second kind of crystal we have made out of this F C C lattice. So, the third kind.

We will start with the F C C lattice, we have put a 2 carbon motif to make a crystal, which is the Diamond Cubic Crystal and this Diamond Cubic Crystal is still called a cubic crystal because, the 3 fold axis has been preserved. So, let us look at the physical model of the Diamond Cubic Crystal and understand the presence of this 3 fold. So, this example, is an ample proof that if 4 fold is lost still you can call a crystal as a cubic crystal.

But, if the 3 fold is lost then you will not or more precisely, if there are no 2 3 folds then such a crystal cannot be called a cubic crystal. So, this is my unit cell of the Diamond Cubic Crystal and you can see that the tetrahedral arrangement has been shown by, this red lines and these, white lines unfortunately there are 2 white lines you will have to focus on the one which are on the cell edges are the once, which are the unit cell edges.

So, you have the tetrahedral order progressing from the central atom to the various atoms. If you look at along the body diagonal, you will see that it has got 3 fold rotational symmetry. So, I will use other camera angle actually, to show this 3 fold rotational symmetry. So, now I am looking at my diamond cubic structure, along the body diagonal which is been positioned from the top. So, now this is my 3 fold direction.

So, I the my 3 fold direction passes, along the body diagonal. The inner or the carbon atoms located within the unit cell them selves forms a tetrahedron and this is along the 3 fold of that tetrahedron as well. So, when I am saying 3 fold axis, what I mean if, I may rotated by 120 degrees I will end up with the same structure. So, again I can rotate by the 120 degrees and I will end up with this same structure. I can do this operation in finite number of way times.

So, this body diagonal of mine is a 3 fold, and any body diagonal of this cube for instance, if I take this body diagonal again would be a seat of the 3 fold axis and it would have all the 4 directions, this body diagonal, this body diagonal all the 4 of them as 3 fold axis. And therefore, in effect to have 4 3 fold axis, which is what is a defining characteristic of cubic crystals, and this crystal I have generated would be called a Diamond Cubic Crystal.

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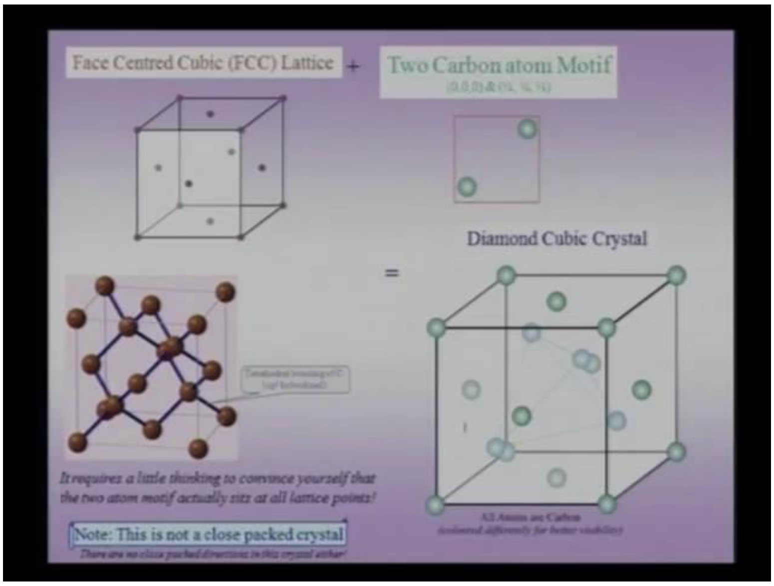

Face Centred Cubic (FCC) Lattice + Two Carbon atom Motif

Diamond Cubic Crystal

=

It requires a little thinking to convince yourself that the two atom motif actually sits at all lattice points!

Note: This is not a close packed crystal

There are no close packed directions in this crystal either!

All Atoms are Carbon

(coloured differently for better visibility)

So, we have pointed out that this axis which is, along the cell edge is not a direction of the 4 fold, but we will see it is related to the 4 fold, but in a different way. So, to summarize this slide about Diamond Cubic Crystals D C. When I say it refers to a crystal, it is a 2 carbon atom motif there, is it is different in bonding characteristics from the sodium chloride crystal which is got ionic bonding while this is a covalent bonded crystal, this is not a closed pack crystal and more importantly I should know, that when I talked about the B C C crystal for instance this was my B C C Crystal.

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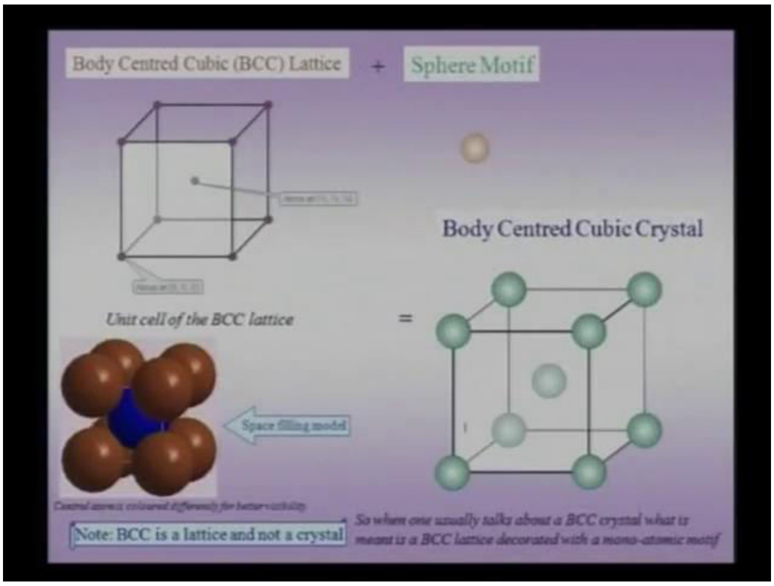

Body Centred Cubic (BCC) Lattice + Sphere Motif

Unit cell of the BCC lattice

Space filling model

Central atoms coloured differently for better visibility

= Body Centred Cubic Crystal

Note: BCC is a lattice and not a crystal

So when one usually talks about a BCC crystal what is meant is a BCC lattice decorated with a mono-atomic motif

This is also not a closed pack crystal, but it still had a closed pack direction and the direction was the direction of the body diagonal. So, we had the case for instance the Face Centered Cubic Crystal which was itself a closed pack crystal, it had closed pack directions, which was along the direction I have shown here. This is the closed pack direction, the face diagonal. So, is a closed pack crystal with, closed pack directions in it. When you went to the B C C we saw that it is not a closed pack crystal, but it still has closed pack directions, which is along the body diagonal of the Body Centered Cubic Crystal.

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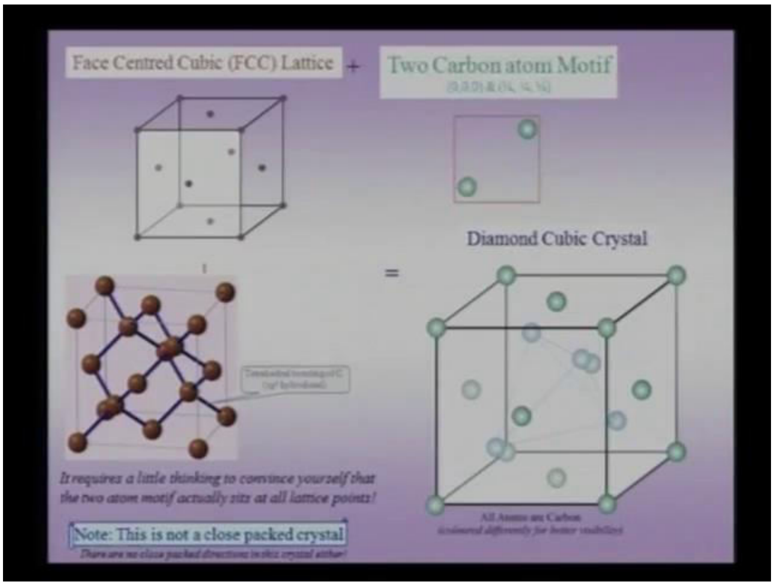

Face Centred Cubic (FCC) Lattice + Two Carbon atom Motif

(0,0,0) & (¼, ¼, ¼)

= Diamond Cubic Crystal

It requires a little thinking to convince yourself that the two atom motif actually sits at all lattice points!

Note: This is not a close packed crystal

There are no close packed directions in this crystal either!

All Atoms are Carbon (coloured differently for better visibility)

Now, we have it with us another example, which is the Diamond Cubic Crystal, which neither is closed pack nor has a any closed pack directions. Because, if I try to travel along the direction of touching which is the body diagonal direction, I see that this atom is touching this atom, but then the next connectivity is from this quarter, quarter, quarter position to a half, half 0 kind of position. So, that continues path of carbon atoms, along the body diagonal is missing and therefore, this kind of crystal is neither closed pack nor has closed pack directions.

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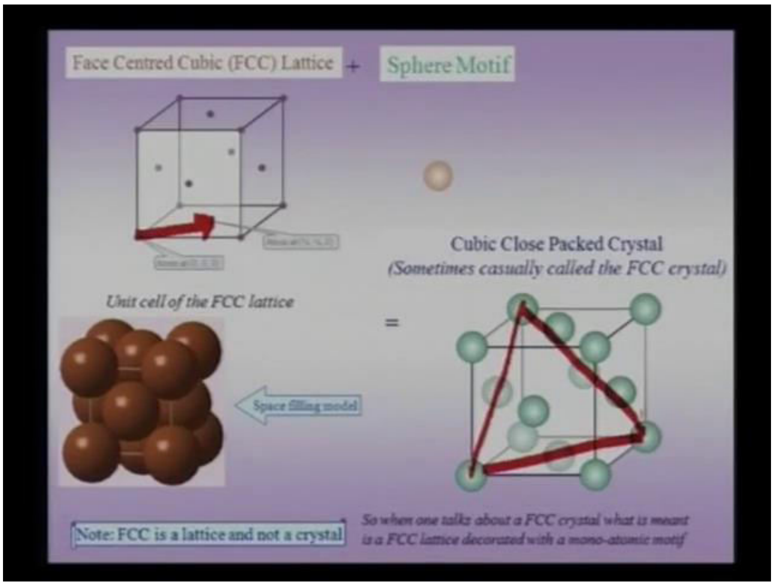

Face Centred Cubic (FCC) Lattice + Sphere Motif

Unit cell of the FCC lattice

=

Cubic Close Packed Crystal
(Sometimes casually called the FCC crystal)

Space filling model

Note: FCC is a lattice and not a crystal

So when one talks about a FCC crystal what is meant is a FCC lattice decorated with a mono-atomic motif

Now, another aspect we could have considered was closed pack presence of closed pack planes. So, for instance when I am talking about F C C Crystal, this is a closed pack crystal, it has got closed pack planes and these, closed pack planes are the we will consider this in a little more detail later for just for being had a little bit now, are these kind of planes which are drawn by, this kind of a plane.

So, will see the miller indices of this plane in later will be the 1 1 1 kind of plane and this, kind of a crystal has is a close pack crystal it has got closed pack planes but, also has got closed pack and in addition it has got closed pack directions. This crystal the Body Centered Cubic Crystal is not closed pack it has no close pack planes, but have got a closed pack direction. This diamond cubic crystal itself is not closed pack it has no close pack planes an addition it has got no close pack directions.

So, we have to remember all these saddle points, that when I am describing crystal we should not only try to identify the structure, how is it closed pack or not closed pack, but in addition we look for these special directions, which are the closed pack directions. Now, we have already seen the symmetry of the crystal can be lowered, if you put a motif which is in a certain way. Now, we will consider some of the examples in 3 dimensions, some of the 2 dimensions analogs of this we have already seen, what happens when I try to put motif which do not have much of symmetry.

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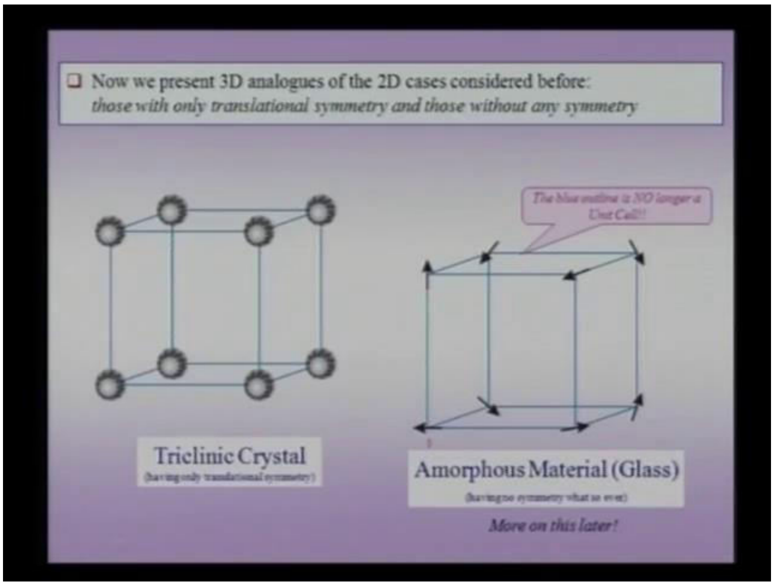

☐ Now we present 3D analogues of the 2D cases considered before:
those with only translational symmetry and those without any symmetry

The blue outline is NO longer a Unit Cell!!

Triclinic Crystal
(having only translational symmetry)

Amorphous Material (Glass)
(having no symmetry what so ever)

More on this later!

For instance the left hand side of this figure is shown a figure, where in I have put a very irregular looking kind of a motif. Typically of course, in nature you will not obtain a motif which looks like this, but typically it could be a combination of many atoms use for instance could be having a molecule a polymeric molecule or any other kind of large molecule with many atoms which has no symmetry in itself.

When I said put such a motif, on this cubic lattice which I started off with, you can clearly see that all symmetry has been lost, except translation. And therefore, the crystal on the left hand side even though it is made above the a simple cubic lattice is a try-clinic crystal and not a cubic crystal. The lattice parameters not affected by this process because, the lattice parameter I assume is the original ideal geometrical lattice parameters, which are a equal to b equal to c Alfa is equal to beta is equal to gamma is equal to 90 degrees.

Now, the figure on the right hand side, I have made by decorating my simple cubic lattice with an shape of an arrow but, now I have not put this arrow in a single orientation. So, in other words going from 1 point to the other, I just rotated my arrow any way I like. So, in when I go across this 3 dimensional space in a finite lean x y is a direction I going to putting this arrows, in ways orientations.

Now, we have to remember what I obtain by, doing this process like, in we saw in the case of the 2 dimensional version of this, the final product I obtain is actually not a crystal it is amorphous. In this blue outlines originally, which formed the unit cell of the lattice is no longer a unit cell of the crystal because, I am not a pennial crystal by this process. We shall see that how can we like, I pointed in the case 2 dimensional version of this, that how we can deal with these kind of crystals or this amorphous structures, with in a frame of crystallography we will consider this a little later.

So, we have to remember that because, we have start with a cubic lattice I do not have to land up either with a crystal with the highest symmetry, which is 4 by m 3 bar 2 by m symmetry or in extreme cases I can even land up with triclinic or amorphous materials, even starting with the cubic lattice. I could of course, started with this Body Centered Cubic lattice or a Face Centered Cubic lattice, but for simplicity, I choose a simple cubic lattice.

Now, there is an this is, perhaps the some important slides we are going to consider next, and the importance of these slides is because, so far what we have been doing is what is called mathematical crystallography. And of course, we extended the mathematical crystallography little bit by, putting these kind of atomic motifs, like the carbon motif, 2 atom carbon motif, for the sodium and the chlorine ions or for instance in the F C C case we could have chosen a carbon copper or a zinc or any of these atoms species for the F C C case I would choose copper or nickel.

And as, you know when it forms a metallic bond then you will have copper or nickel ions which will decorate the F C C lattice to give you a copper crystal or a nickel crystal. So, there has to be absolute distinction between, the ideal mathematical crystals and real crystals. And some of this examples, we have considered should not mislead you to thinking that in nature there is no connection between, the symmetry and the geometry.

So, the coming slide will explain to you that actually, in real practical example, especially in atomic examples, we could have a connection between the geometry and the symmetry in other words, when I put a lower symmetry motif on to higher the symmetry lattice. It could, so happen that the lattice itself will undergo a distortion because, of the atomic entities would repel or attract each other, the usual bondings. And it can lead to a different kind of a crystal which would be consistent; that means, the lattice would become or the geometrical aspect would become consistent with the symmetry aspects.

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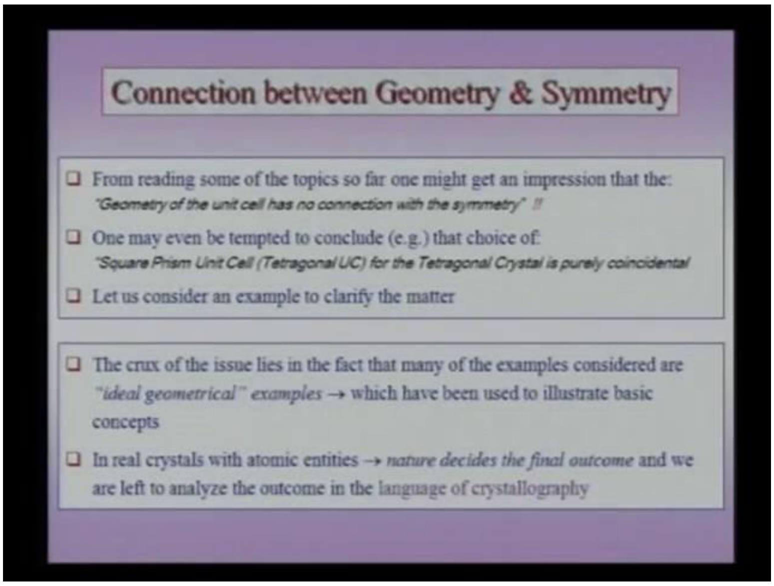

Connection between Geometry & Symmetry

- ☐ From reading some of the topics so far one might get an impression that the: *"Geometry of the unit cell has no connection with the symmetry"* !!
- ☐ One may even be tempted to conclude (e.g.) that choice of: *"Square Prism Unit Cell (Tetragonal UC) for the Tetragonal Crystal is purely coincidental*
- ☐ Let us consider an example to clarify the matter

- ☐ The crux of the issue lies in the fact that many of the examples considered are *"ideal geometrical" examples* → which have been used to illustrate basic concepts
- ☐ In real crystals with atomic entities → *nature decides the final outcome* and we are left to analyze the outcome in the language of crystallography

So, to state the important point from reading some of the topics, so far 1 might get an impression, that the geometry of the unit cell has no connection with the symmetry. It can happen in ideal mathematical crystals or crystals which we make some of the natural crystals. There will be a connection more often than not, one may even be tempted to conclude that the choice of for instance, the square prism unit cell tetragonal unit cell for the tetragonal crystal is purely coincidental such a choice may you might purely coincidental. Let me consider one example at this point of time to clarify the matter. So, mister Patel has a question.

Student: I have one question that were related to just before slides for maximum closed packing there is a close pack fraction is 74 percent if we choose a same one type of motif and for N a C l we take here 2 types of motif and here close packing is reduced. So, how we can define any crystal is closed pack or not. You just taken some plains or direction in the closed packing. So, I want to clarify just we can (Refer Time: 33:59)

Very, very, very important question now, mister Patel's question is that I started with the single sphere motif and obtained the closed pack structure which had a packing fractional 74 percent. Now, how do I conclude that a given crystal is closed packed or not the first thing we saw the requirement, was the existence of spherical atoms. Now, we could have atoms whose electronic density in outer level could be very different from spheres and they may not behave like an ideal closed pack spheres and therefore, the packing fraction become down from ideality.

Later, when we consider hexagonal closed pack crystal we will see that this could be an important issue because, often, more often than not then ideal closed packing of in hexagonal format would give you an ideal c by ratio, but we will see that most real crystals deviate from this ideal c by ratio, which means they deviate also from the ideal packing fraction which we assume.

Now, what is the criteria that we understand that has to be closed pack or not it is the packing fraction suppose I calculate my packing fraction it is less than 74 percent which is the theoretical maximum then I would conclude that it is not a closed pack crystal, I will not be bios my conclusions either on the presence of closed packed directions or the presence of closed packs plains it will purely based on the volume closed packing, which mean the packing fraction of space.

So, this is the very important question to be kept in mind and perhaps will take of an hexagonal closed pack another crystals this may become more obvious. So, coming back to the connection between geometry and symmetry, in real crystals with atomic entities nature decides a final outcome and we are left to analyze the outcome in the language of crystallography. So, there are crystals of we will see some examples which we make ourselves.

We could make crystals for instance out of this big entity out in a hand two more examples will see soon, but there are crystals which are at least even though you make them artificial in the laboratory or may occur naturally in, but there may be assembled by themselves. But, in the case if nature or an artificial size crystal is made then it is our job to analyze the outcomes in terms of the language of crystallography. So, it is not that in every case, we can make a crystal starting with any kind of motif or any kind of entities sometimes the nature decides what will be the outcome. So, let me consider the one example to connect my geometry with symmetry.

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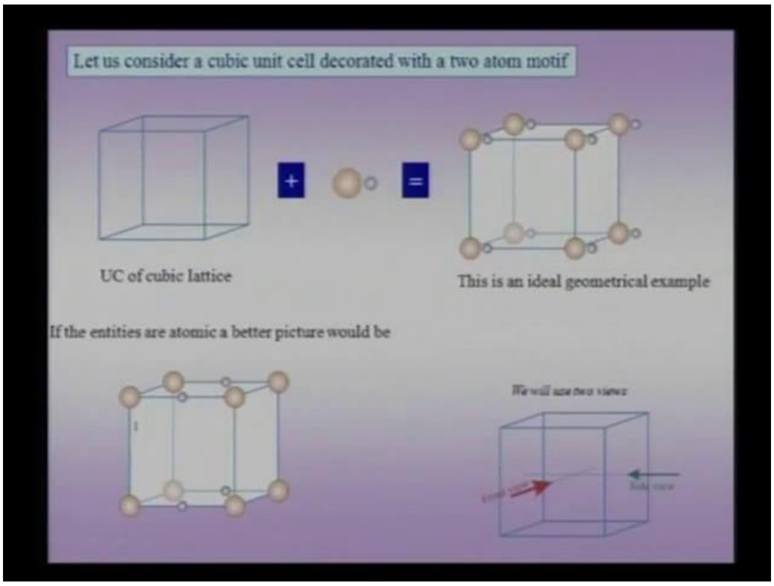

Let us consider a cubic unit cell decorated with a two atom motif

UC of cubic lattice

This is an ideal geometrical example

If the entities are atomic a better picture would be

We will use two views

So, for instance now, I take a unit cell of a cubic lattice and now, I assume that these are 2 atomic entities, real atomic entities for, now. If I now, decorate this lattice with this atomic entity it is now, my motif I will get a structure like this. Now, there is no reason assumed that the way I am drawing it that this should not sit in the centre. So, an alternate we are drawing the same thing is that there is a orange sphere and gray sphere and they will sit like this in unit cell. Now, let me use two views to understand this kind of a crystal I will use a front view and I will use a side view. So, I start with a simple cubic lattice I put a two atom motif and the structure I obtain like this which I shall understand with two views.

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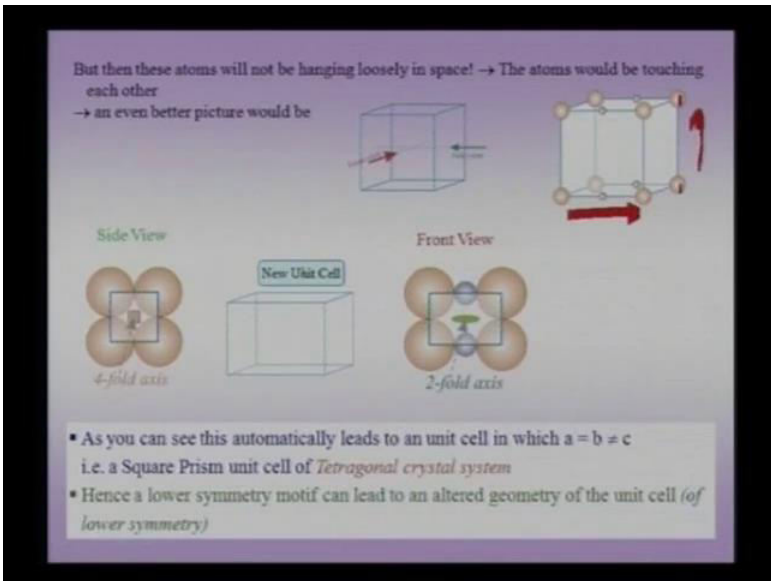

But then these atoms will not be hanging loosely in space! → The atoms would be touching each other

→ an even better picture would be

- As you can see this automatically leads to an unit cell in which $a = b \neq c$
  i.e. a Square Prism unit cell of *Tetragonal crystal system*
- Hence a lower symmetry motif can lead to an altered geometry of the unit cell *(of lower symmetry)*

Now, what would happen to this arrangement typically, you would see that because, there is additional entity here, this direction would be for instance this direction, would have a longer length as compared to this direction where my atoms this atom can actually touch this atom. So, if I look at for instance the front view I would see a configuration like this. So, there will be an atom here, there will be a gray and there will another orange.

So, I will see that this shape will turn into a rectangle, while this atom is touching each other. So, this is the shorter length, if I look from the other direction which is the side view I will see that actually, I can see a 4 fold axis and the 4 atoms would be touching each other. So, what is a resultant the resultant would be a new kind of an unit cell which I have shown the centre here.

Therefore, the conclusion from this exercise is that when I put motifs of lower symmetry then the typical unit cell will also lower down to that kind of a to adjust that kind of a motif and therefore, there will be no conflict between the symmetry and the geometry. So, now this is a unit cell of the tetragonal crystal, the crystal itself has a tetragonal symmetry; that means, has got only one 4 fold axis the 3 axis remain orthogonal; that means, alpha is equal to beta is equal to an gamma is equal to 90 degrees.

So, this is a perhaps simplistic example, but never the less brings out the important point, that the kind of motif we have put automatically leads to an unit cell in which a is not equal to a is equal to b, but not equal to c and the unit cell we have squared represent that of the tetragonal crystal system. And hence, the lower symmetry of the motif can lead to an altered geometry of the unit cell of lower symmetry, in other words the common shape of unit cell you would see in text books, in other words many text books will mention the tetragonal crystal would mean a is equal to b is not equal to c alpha beta gamma is equal to 90 degrees.

And there is usually no mention of the symmetry aspect, but you can see from this example, that the symmetry and the geometries are of coincide with each other and the language become consistent at least in these kind of atomic entities. After making crystals in one 2 and 3 dimensions.

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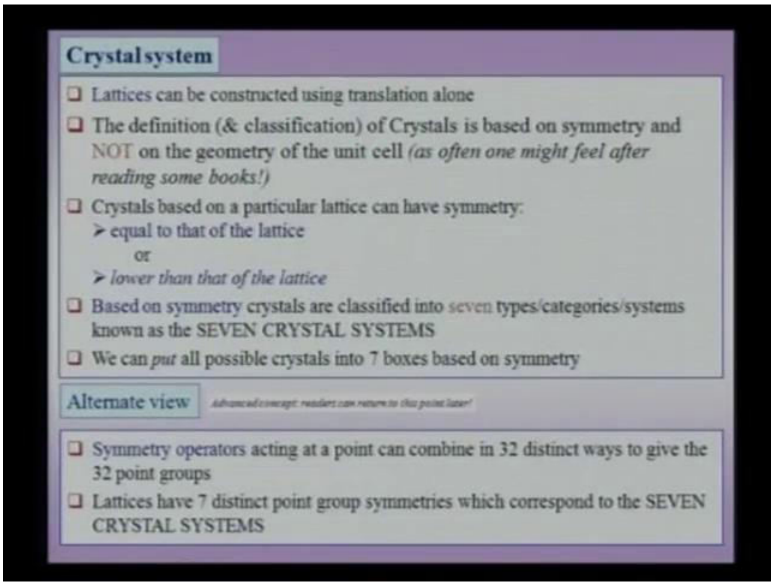

Crystal system

- ☐ Lattices can be constructed using translation alone
- ☐ The definition (& classification) of Crystals is based on symmetry and NOT on the geometry of the unit cell *(as often one might feel after reading some books!)*
- ☐ Crystals based on a particular lattice can have symmetry:
  - ➢ equal to that of the lattice

    or
  - ➢ *lower than that of the lattice*
- ☐ Based on symmetry crystals are classified into seven types/categories/systems known as the SEVEN CRYSTAL SYSTEMS
- ☐ We can *put* all possible crystals into 7 boxes based on symmetry

Alternate view Advanced concept: readers can return to this point later!

- ☐ Symmetry operators acting at a point can combine in 32 distinct ways to give the 32 point groups
- ☐ Lattices have 7 distinct point group symmetries which correspond to the SEVEN CRYSTAL SYSTEMS

Let us now, return to our main flow which is considering the various crystal systems. This may be a good point to revise some of the aspects perhaps not in detail, but a little revision. So, we have seen lattices can be constructed using translation alone the definition of crystals is based on symmetry and not on the geometry of the unit cell and we have seen that often these 2 coincide or they can coincide at least in the case of some real crystals.

Crystals based on the particular lattice can have symmetry equal to that of the lattice or lower than that of the lattice based on symmetry, crystals are classified into 7 types known as the 7 crystal systems, we will take up the 7 crystal systems one by one very soon. We can put all possible crystals into 7 boxes which we call the 7 crystal systems. In advanced kind of consideration at this point of time, but it might sort of enthuse you to go and read about these kind of aspects in a more detailed text like from elementary crystallography burger.

And the points I mentioned are symmetry operators, acting at a point in combined in the 32 distinct ways, to give the 32 point groups lattices have 7 distinct point to symmetry which correspond to the 7 crystal systems. So, there is a very sound bases of why we should have 7 crystal systems that absolutely clear. So, the important points to highlight are the point which is been outlined in this doted box.

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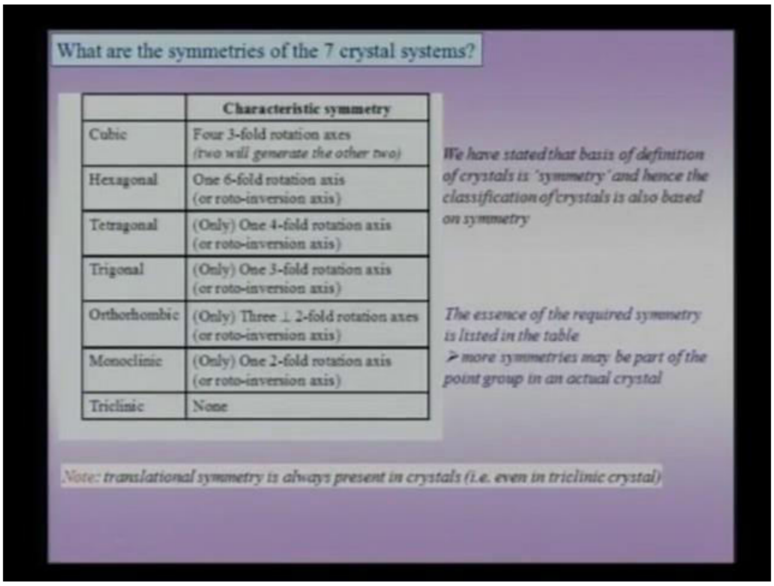

What are the symmetries of the 7 crystal systems?

	Characteristic symmetry
Cubic	Four 3-fold rotation axes *(two will generate the other two)*
Hexagonal	One 6-fold rotation axis (or roto-inversion axis)
Tetragonal	(Only) One 4-fold rotation axis (or roto-inversion axis)
Trigonal	(Only) One 3-fold rotation axis (or roto-inversion axis)
Orthorhombic	(Only) Three ⊥ 2-fold rotation axes (or roto-inversion axis)
Monoclinic	(Only) One 2-fold rotation axis (or roto-inversion axis)
Triclinic	None

We have stated that basis of definition of crystals is 'symmetry' and hence the classification of crystals is also based on symmetry

The essence of the required symmetry is listed in the table

➢ more symmetries may be part of the point group in an actual crystal

Note: translational symmetry is always present in crystals (i.e. even in triclinic crystal)

Now, we have to ask this obvious question that, since we are now talking about crystals the definition of crystals based on symmetries. So, we have to ask what are the symmetries to the 7 crystal systems, in other words what is the characteristic symmetry of all the 7 crystal systems for instance, we have already seen that cubic crystals need to have 2 3 fold axis. So, the cubic crystal needs to have 4 3 fold axis which can gives start with 2 and the remaining 2 would be generated automatically external crystal has one and only 1 6 fold rotation axis.

And it is important point to note, since we are now talking about crystals it is not necessary that the 6 fold need to be a regular 6 fold, it could be an alternate form for instance it could be a roto-inversion axis or a screw axis as well. So, other kinds of symmetry operators which have 6 in them need to be present at least one of them need to be present. The tetragonal crystal for instance has only one 4 fold axis.

If there are two 4 fold axis then; obviously, it goes into the cubic class, this 4 fold again like the 6 fold need not be a pure normal rotation axis, but could be actually a roto-inversion axis. The trigonal crystal has only one 3 fold rotation axis and of course, as before it could be a roto-inversion axis. So, if it had two 3 fold axis it will come under the cubic class it has only one 3 fold axis it will come under the trigonal class and we have seen an alternate name for this trigonal it is also called the robohedral crystals.

But, I prefer the term trigonal because, the word tri refers to the 3 folded unless which is the symmetry of the crystals coming under this class. Now, we also did this operation where in we started with the cube and pulled it along the body diagonal which may the operation was such that it retained it is one 3 fold axis and destroyed the other 3 fold axis. So, we saw that how we can start from a cubic kind of an unit cell and go to the trigonal kind of an unit cell which is otherwise called the rhombohedral unit cell.

The ortho-rhombic crystals have three 2 fold rotation axis perpendicular to each other. This could of course, also be roto-inversion axis, and we will actually list down the point groups which would go in this ortho-rhombic class of crystals. The mono-clinic crystal on the other hand only one 2 fold axis which could also be a roto-inversion axis. The crine tri-clinic crystal has no kind of symmetry except translational symmetry; however, we can write it as, a one fold symmetry or a one bar symmetry in other words you can still call it have the crystal having a one bar symmetry under come under the tri-clinic class.

So, even though we say no symmetry we actually, mean that it has got translation symmetry and in addition we could have an one bar symmetry. So, this point has to be kept in mind regarding tri-clinic crystals. So, of course, one fold symmetry itself is a trivial thing to describe but, one bar is slightly not, so trivial and similarly, translation is definitely left in the tri-clinic crystals. We have listed in this table for instance, the very essence of the symmetry which needs to be present in these various classes. A more symmetry is could be present part of the point group and we will list them one by one when we soon consider the 7 crystal systems. So, we have the 7 crystal systems 1 2 3 4 5

6 7 and these are the characteristic symmetry of these crystal systems. And then complete elaborate point group symmetries will be written in the coming slides.

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THE 7 CRYSTAL SYSTEMS

So, let us now, consider the 7 crystal systems one by one.

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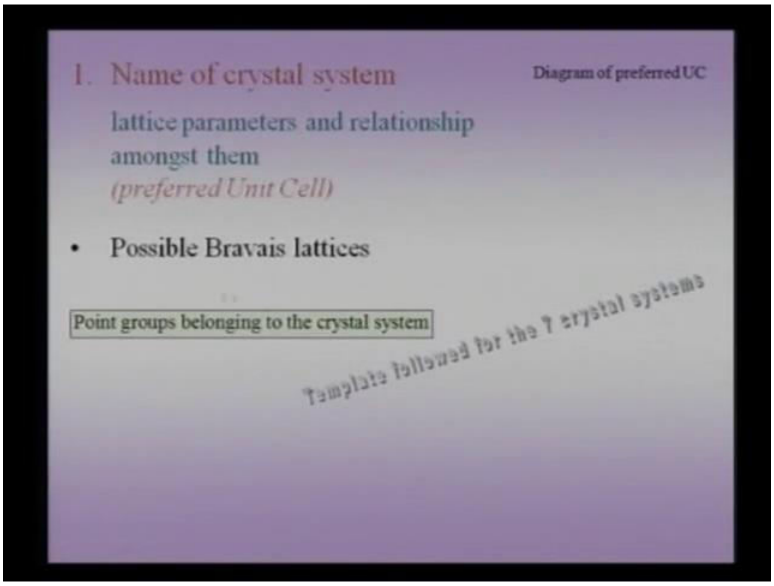

1. Name of crystal system

Diagram of preferred UC

lattice parameters and relationship amongst them

(preferred Unit Cell)

- Possible Bravais lattices

Point groups belonging to the crystal system

Template followed for the 7 crystal systems

When we consider these crystal systems I will use the following template I will use the Name of the Crystal systems I will use the typical choice of the unit cell and the lattice parameters describing that unit cell. I will also show a diagram of the preferred unit cell, I will also list under the crystal system the Possible Bravais lattice from which they have been constructed I will put down the point groups belongs, to this crystal system. And in at least the cubic case I will show you additionally the shape of these crystals which is a very important concept. So, this is my template for describing the 7 crystal systems.

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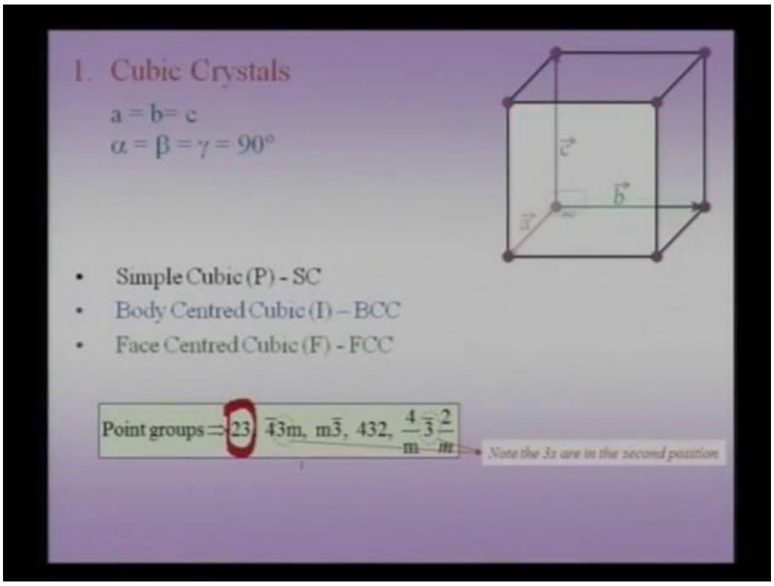

1. Cubic Crystals

$a = b = c$

$\alpha = \beta = \gamma = 90^\circ$

- Simple Cubic (P) - SC
- Body Centred Cubic (I) – BCC
- Face Centred Cubic (F) - FCC

Point groups ⇒ 23, $\bar{4}3m$, $m\bar{3}$, 432, $\frac{4}{m}\bar{3}\frac{2}{m}$

Note the 3s are in the second position

So, let me start with the simplest or the, high symmetry one which is cubic crystal. We know these interrelationship between the lattice parameters from before and this is how my unit cell of a Cubic Crystal typical choice would like you already seen from previous examples, that these are the possible bravi lattices which from, which you can construct a Cubic Crystal. And now, there is something slightly more sophisticated which is the listing of the point groups.

Though from an elementary course point of view it is may not be necessary to remember each one of point groups, but some of the essence need to be noted for instance I mention that a Cubic Crystal needs to have this two 3 fold axis, which would of course, result in four 3 fold axis. So, if at all I am writing down a point group of a Cubic Crystal you will see that the 3 appears in the second place.

So, everyone of these point groups there is a 3 the second place of course, it may not be a normal 3 it could be a three bar which we have also pointed out in the slide which we had considered here that it did not be a pure rotation axis it could be a for instance roto-inversion axis. Now, this is listing also brings to you the other important point, that when

I had a cubic lattice it had the highest symmetry which I call the holohedral symmetry of this crystals.

So, the cubic lattice and some of the Cubic Crystals which I can construct and have this highest symmetry, which is the one written on the right hand side, but it could also have some of the lower symmetry, once for instance this 2 3 is a is a possible symmetry of Cubic Crystals. And when we are mentioned the concept of space filling, we had considered that though on one hand there is a concept of space filling and there is a close association of the concept of space filling, with crystals by other concepts of the unit cell, but we should never confuse the concept of space filling with the presence of symmetries.

And this is a very good example to show this the 2 3 symmetry, for instance tetrahedra do not fill space, but 2 3 symmetry which is tetrahedral symmetry, is allowed in crystals, and more precisely it is allowed in classified under the cubic crystals. So, this has to be absolutely clear at this point of time. Another point worthwhile to note is that for instance 4 by m 3 bar 2 by m kind of a crystal would have a centre of inversion. While a crystal having a 2 3 symmetry will not have a centre of inversion.

In other words if I am looking at the property, which has a symmetry exactly equal to that of the point group of the crystal. In that case up if you invert the direction the properties need not be invert because, just because, for instance in such a crystal with 2 3 point group the 1 0 0 direction will or the positive x direction will not be equal to the negative x direction. So, that has to be remembered because, a crystal does not have a centre of inversion. So, it is very important for me to understand not only that what lattice a crystal starts off with, but what is the exact point group symmetry of the crystal in order for me to correlated with the properties one of the important properties I may look out for is the shape of the crystal.

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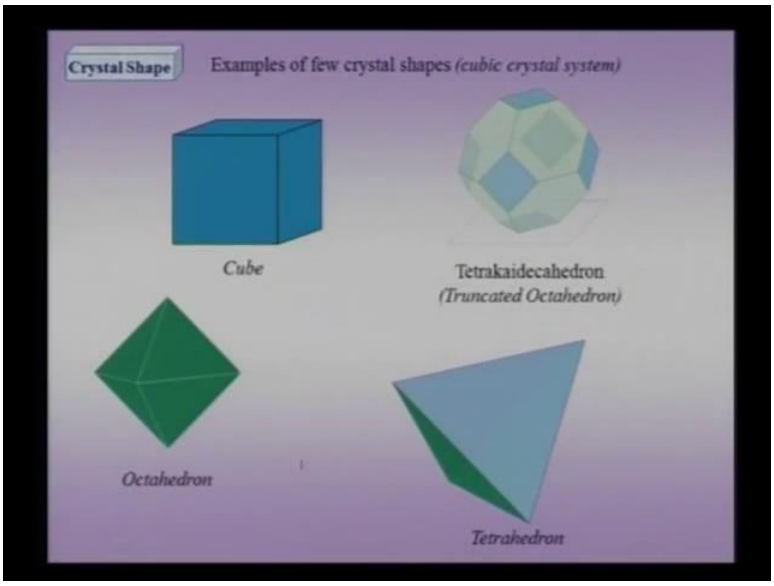

Crystal Shape

Examples of few crystal shapes *(cubic crystal system)*

So, for instance I am now, considering what is known as the well grown crystal which is otherwise, known as the euomorhic crystal.

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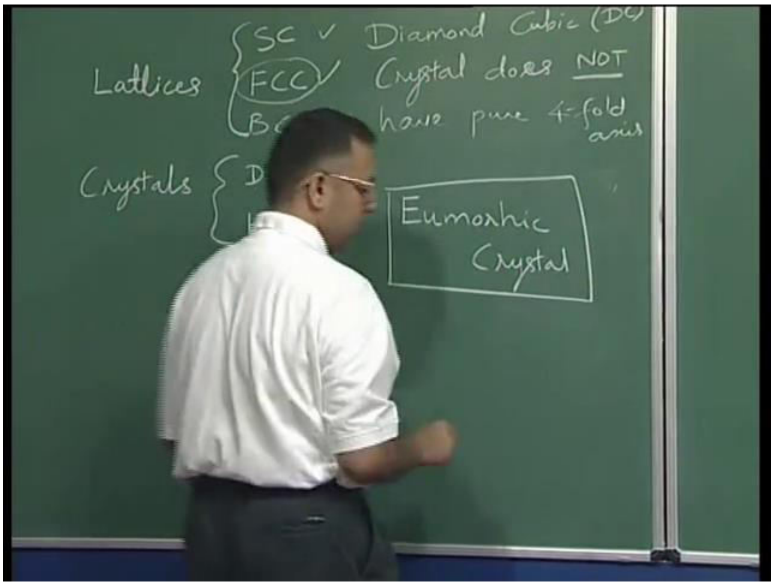

So, when I grow a crystal and of course, I will assume that the energetic determine the shape of the crystal; that means, the outer shape is well formed, then cubic crystals will typically grow, under grow in various shapes I mean go or more importantly let me consider equilibrium shape for now; that means, that the outer shape is an equilibrium shape of the crystal.

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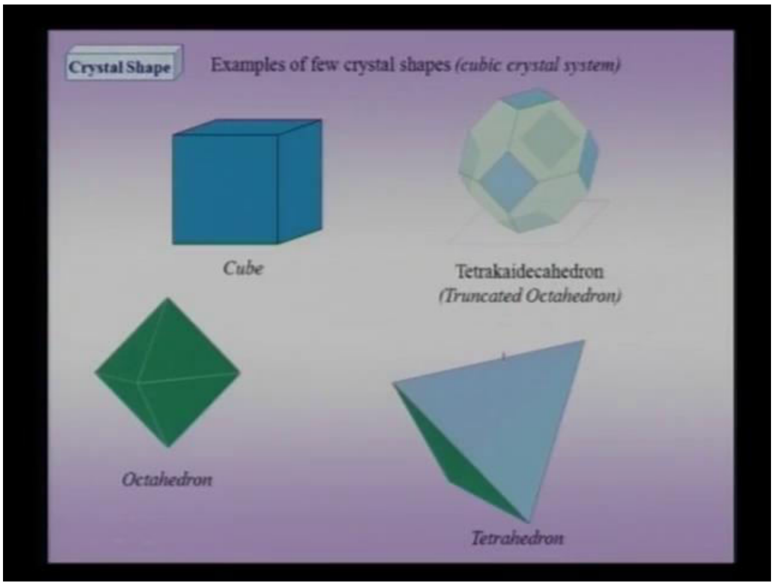
Crystal Shape

Examples of few crystal shapes *(cubic crystal system)*

But, more importantly, what I need to know that the equilibrium shape of the crystal for instance for the cubic crystals could be a cube or an octahedron or for instance this is a truncated octahedron which is known as the tetrakaidecahedron, and we have seen previously that this tetrakadecahedron is a space filling solid. Now, it could grow in one of these 3 shapes or many, many other shapes which have between all these shapes.

So, this is let me repeat this important point, for a crystal if it is been well formed and it is equilibrium shape; that means, the global energy minimize shape I am considering a finite crystal. Then the outer shape of the crystal for a cubic class would say, for instance now, I am considering the highest cube symmetry once for instance 4 by m 3 bar 2 by 3 symmetry once, would could be not just a cube because, tell would have a shape which is an shape of an octahedron as well it would also have a shape of the tetrakadecahedron.

And here in is an important point to note that the external shape reflects the inner symmetry present in a crystal. So, far we were dealing with, the mathematical crystallography, the language of crystallography in a pure mathematical sense, but now we are talking about a very practical aspect a properties of crystals and we will mention something more about properties of crystals very soon.

And when we talk about properties of a crystal, we have to remember for instance this is one property the shape of a crystal, that reflects the inner symmetry of the crystal of course, the crystal has to be well form and sometimes it is very difficult to get these well formed crystals. So, and it mean for instance the higher symmetry cubic crystal need not just be a form of a cube the external shape could be the shape of an octahedron. So, that has to be remembered and this is where there is a confluence of the concept of mathematical crystals and real crystals.

Even though, we have a spoken a language of point group symmetries etcetera, but now we have a physical crystal which in some way is that is where the joining of the both the concepts in mathematical and the physical where takes place and this is one of the properties, joining would also takes place in many other ways, in many other properties, but this a beautiful example, and before even for instance the formal mathematical language of crystallography, developed people have been observing that crystals actually grow in shape.

And this is been some of the reason of quite a bit of interests mineralogists, in crystals is the beautiful shapes they would grow under and some of the beautiful optical properties, the shapes would lead to. And, so we can see that these crystals can grow in these shapes, a load symmetry tetrahedral crystal for instance could grow in the shape of a tetrahedron. There many, many more shapes taken grow in, but for instance for you to remember for now, is that the external shape reflects the inner symmetry. That is an important point to be noted down. So, let me write this down on the board.

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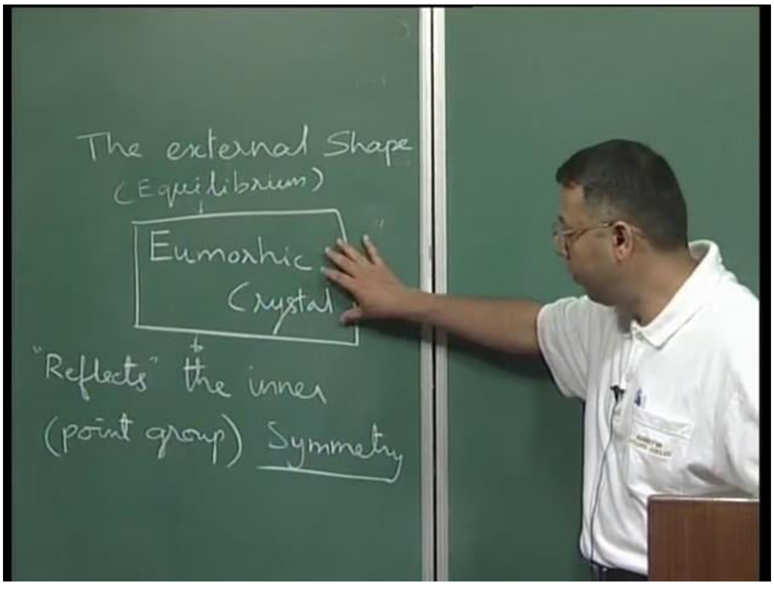

The external Shape
(Equilibrium)
Eumorhic
Crystal
"Reflects" the inner
(point group) Symmetry

External shape of eumorphic crystals. So, the external shape of for I considering equilibrium crystal of a well grown or eumorhic crystal, reflects the inner point group symmetry of the crystal. So, once again to warn you just because, I am using the word cubic crystal it does not mean the shape of the crystal has to be cubic, it could be one of the other shapes which has the same symmetry.

In this case just as a warning to advance readers that, we do not consider space group symmetries because, space groups additionally have translations. So, at the scale we are talking as a macroscopic scale and not the macro scale and these translations are at the micro scale and they, are not typically considered which in these macro shapes. So, in the translations order of the atomic translation vectors or lattice translation vectors.

While this shape is the macro scale which could be the crystal or it could be grown as big as my hand or typically, of centimeters and therefore, this the macro scale and therefore, I can ignore the space group symmetries which have translations in them, and all I need to consider at this stage is the point group symmetry. So, this is what I wrote down on the board.

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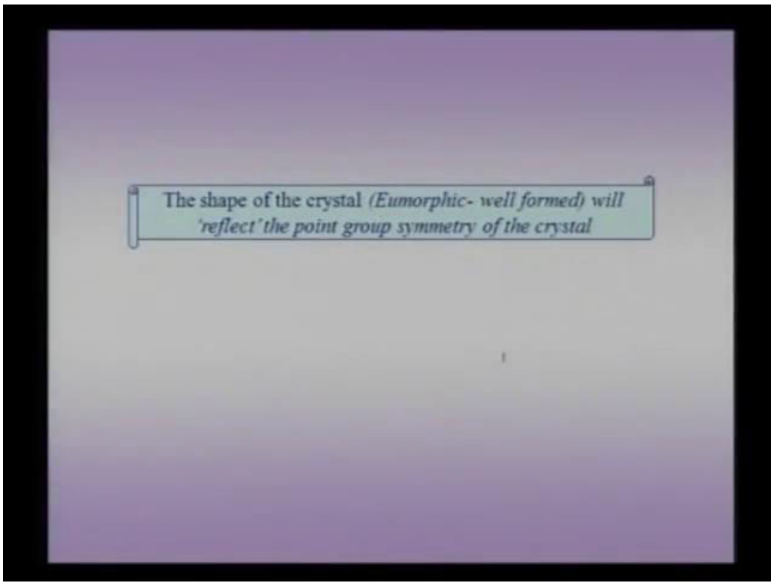

The shape of the crystal *(Eumorphic- well formed) will 'reflect' the point group symmetry of the crystal*

So, just to emphasis this point again the statement is right here for you. Now, which we will see some more points regarding properties of crystals and we will state an important principle very soon.

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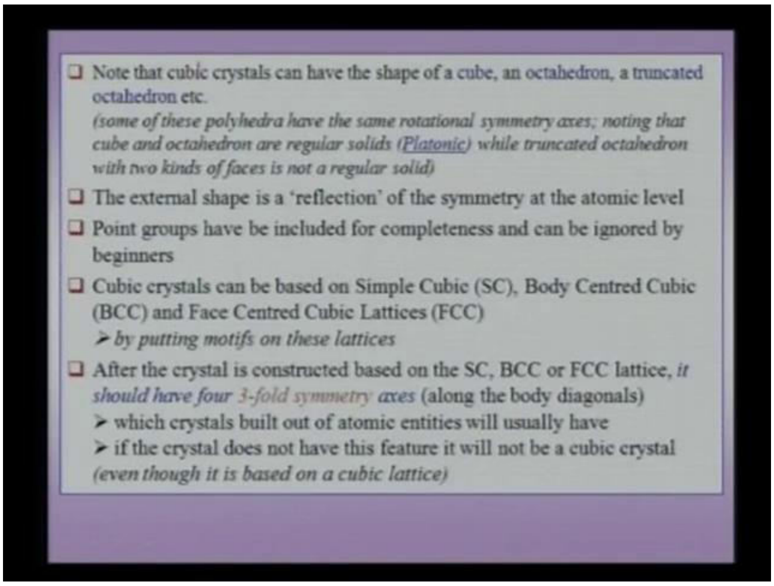

- ☐ Note that cubic crystals can have the shape of a cube, an octahedron, a truncated octahedron etc.
  (some of these polyhedra have the same rotational symmetry axes; noting that cube and octahedron are regular solids (Platonic) while truncated octahedron with two kinds of faces is not a regular solid)
- ☐ The external shape is a 'reflection' of the symmetry at the atomic level
- ☐ Point groups have be included for completeness and can be ignored by beginners
- ☐ Cubic crystals can be based on Simple Cubic (SC), Body Centred Cubic (BCC) and Face Centred Cubic Lattices (FCC)
  - ➢ *by putting motifs on these lattices*
- ☐ After the crystal is constructed based on the SC, BCC or FCC lattice, *it should have four 3-fold symmetry axes* (along the body diagonals)
  - ➢ which crystals built out of atomic entities will usually have
  - ➢ if the crystal does not have this feature it will not be a cubic crystal *(even though it is based on a cubic lattice)*

So, let me summarize the important points regarding some of the aspects of cubic crystals you have considered, we have seen that cubic crystals can have a shape of an cube or octahedron truncated octahedron or many other possible shapes. You have to know that some of these polyhedra have same rotational symmetry axis, noting that cube and octahedron are regular solids platonic while truncated octahedron with two kinds of faces is not a regular polyhedron.

You have seen that the external shape is a reflection of the inner symmetry, at the atomic level. If you find it uncomfortable to work with point groups please ignore them at this stage, but remember that point groups symmetry is nothing, but, a combination of some of these symmetry elements. Cubic crystals can be based on the simple cubic body centered cubic or the face centered cubic lattices by, putting motifs on these lattice. After the crystal is constructed based on these lattices it should have still 3 fold symmetry if it has to come under the cubic class.

Which usually crystals built out of atomic entities have, if the we also seen that crystal does not have this feature it is not logical to classify it under the cubic class. So, I have certain models of cubes here, which have been cut along various directions and this models often now, I will used to demonstrate the fact that, how what you might call the shape of crystal or the faces which are developed in the crystal.

If a crystal has only these kind of a faces for instance now, this is a simple cubic crystal. Then it could have only these kind of faces in which case it will have a shape of a cube, but it could have a combination of these kind of faces and these faces which is now, been truncated along the 1 1 1 direction. So, you can see that if I look at this face it has got a certain atomic density. The on the other hand this face like this, has a lower atomic density in the case of the simple cubic crystal.

The crystal for instance there is another alternate model of the same simple cubic crystal, could have through could have would show faces which are of this type the face I you can see clearly, that has been cut along and you can see that this faces could also be developed and these faces also as you can see have a lower atomic density than the faces of this type, where in all four atoms are touching each other, while in this direction when we cut a plain like this you can see that, atoms are touching along this direction, but not along this direction. So, of course, just the atomic density will not determine the equilibrium shape of a crystal, equilibrium shape of a crystal typically is constructed by a method is known as the wolf construction, but there in we construct the energetic; that means, what is the energy of all these faces.

And if the lowest energy happens to be for the one this kind of a cubic faced and cubic shape, if it happens to be for lowest energy singly for instance for this kind of a face crystal could show an octahedral kind of a shape or there could be a more complicated shape in which you could have these kind of faces which is also this kind of a face, this kind of a face and this kind of face. So, there could be combination of various kind of faces which could develop and that would determine form or the external shape of the crystal.