Structure of Materials
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Lecture - 11
Geometry of Crystals: Symmetry, Lattices

Tetragonal crystals, there are two kind of bravos lattice servicing, the simple tetragonal lattice and the body cantered tetragonal lattice.

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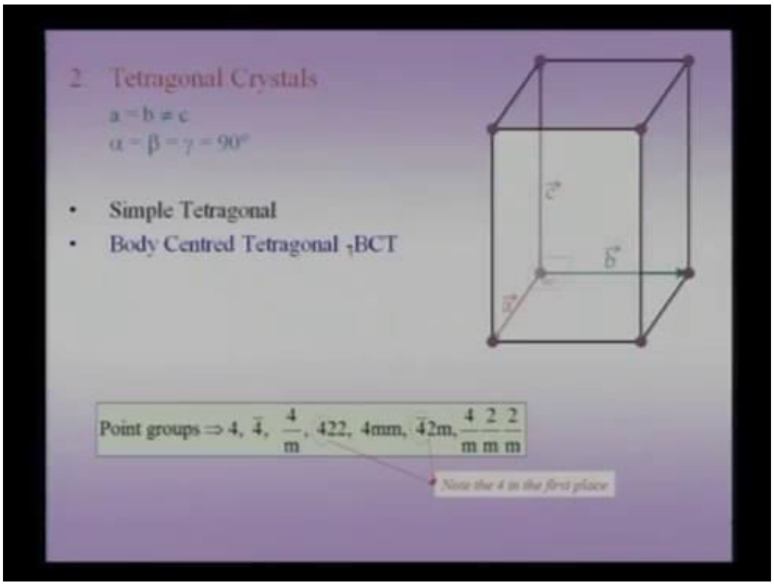

2. Tetragonal Crystals

$a = b \neq c$

$\alpha = \beta = \gamma = 90°$

- Simple Tetragonal
- Body Centred Tetragonal -BCT

Point groups $\Rightarrow 4,\ \bar{4},\ \frac{4}{m},\ 422,\ 4mm,\ \bar{4}2m,\ \frac{4}{m}\frac{2}{m}\frac{2}{m}$

Note the 4 in the first place

The important point to note about tetragonal crystals is the presence of one and only one 4 fold axis of course, this could be a proper 4 fold axis or it would be a 4 bar kind of an axis, which is a rotor inversion axis. Now, if you write down the all the point groups you will notice that the 4 is in the first place in all these point groups, the lattices which have the highest symmetry.

That means, tetragonal lattices always have this 4 by m, 2 by m, 2 by m symmetry, while crystals based up on these lattices could have lower symmetry. And those includes the 4 bar 2 m, the 4 mm, the 422 the 4 by m 4 bar and 4 point groups, we already seen that the preferred unit cell is described by these lattice parameters for the tetragonal crystals.

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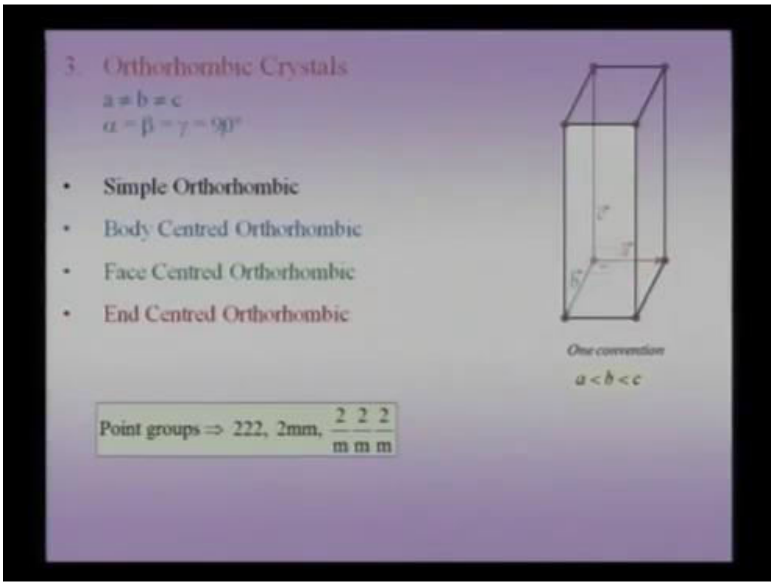

3. Orthorhombic Crystals

$a \neq b \neq c$

$\alpha = \beta = \gamma = 90°$

- Simple Orthorhombic
- Body Centred Orthorhombic
- Face Centred Orthorhombic
- End Centred Orthorhombic

Point groups ⇒ 222, 2mm, $\frac{2}{m}\frac{2}{m}\frac{2}{m}$

One convention

$a < b < c$

The low symmetry one compared to tetragonal crystal is the orthorhombic crystals, where in we see that there are all possible bravail lattices for the orthorhombic case, the simple orthorhombic, the body centred orthorhombic, the face centred orthorhombic and the end centred orthorhombic lattice. So, we can make crystals starting with these kind of lattices, and the point groups which belong to this orthorhombic crystals are the ones listed below the 222, the 2 mm the 2 by m, 2 by m, 2 by m point groups.

All orthorhombic lattices or any one of these 4 would always have a highest symmetry, which would be a 2 by m, 2 by m, 2 by m symmetry, while crystals based on these lattices could have a lower symmetry, which could be a 222 or a 2 mm symmetry. And we also seen that one convention which is typically used to describe the unit cell is where in a in less than b is less than c. And we already noticed that this is the inter relationship among the lattice parameters for the orthorhombic crystals this is; obviously, for the preferred unit cell. And; that means, that you can have; obviously, have alternate choice of units cell as well.

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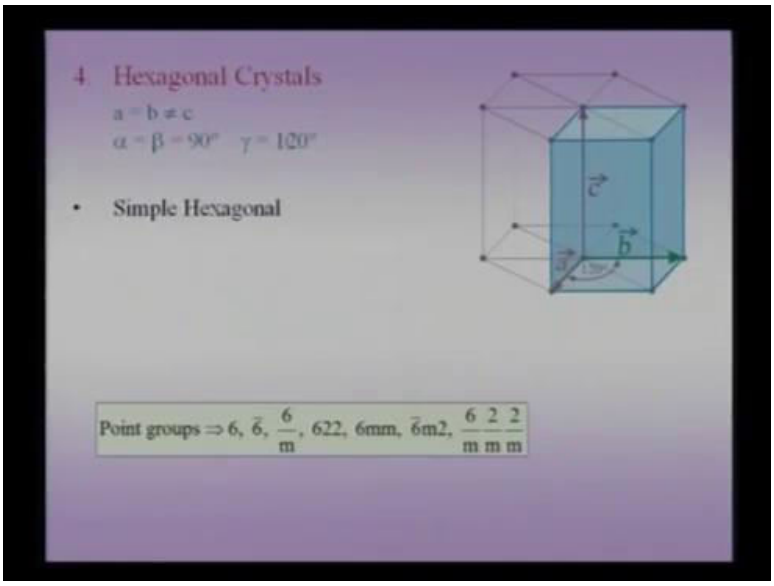

4 Hexagonal Crystals

$a = b \neq c$

$\alpha = \beta = 90^\circ \quad \gamma = 120^\circ$

- Simple Hexagonal

Point groups $\Rightarrow 6, \bar{6}, \frac{6}{m}, 622, 6mm, \bar{6}m2, \frac{6}{m}\frac{2}{m}\frac{2}{m}$

Hexagonal crystals, we have seen are characterized by the presence of a 6 fold or a 6 bar axis, you can see a 6 here, the first place and a 6 here, and a 6 here, and a 6 here and, so forth. So, all hexagonal crystals should have some form of a 6 in the first place in the point group, there is only one kind of lattices as we have seen which is the simple hexagonal lattices. And one of the important crystals the hexagonal closed pack crystals belongs to the hexagonal crystal class. And we will try to understand that crystals in lot of detail in one of the coming lectures.

We already seen the lattice parameters that you c is not equal to a which is equal to b, and the alpha and beta are both 90 degrees and gamma is equal to 120 degrees. So, this is the preferred choice of the unit cells for the hexagonal crystals, and as before the hexagonal lattice always has 6 by m, 2 by m, 2 by m symmetry. While crystals based on this lattice could have one of these lower symmetries, which includes a 6 bar m 2, a 6 mm, a 622, a 6 by m, a 6 bar or a 6.

In other words, there are quite a few point groups which belong to the hexagonal crystals class, and crystals belongs having any one of the symmetries would come under the hexagonal crystal class. The important point to note is that unlike the two dimensional case, where the presence of a 6 fold or a 3 fold a singular 6 fold or 3 fold both came under the 120 degree rhombus class, here the single 3 fold cases are excluded from the hexagonal class, they come under a separate class which is the trigonal class.

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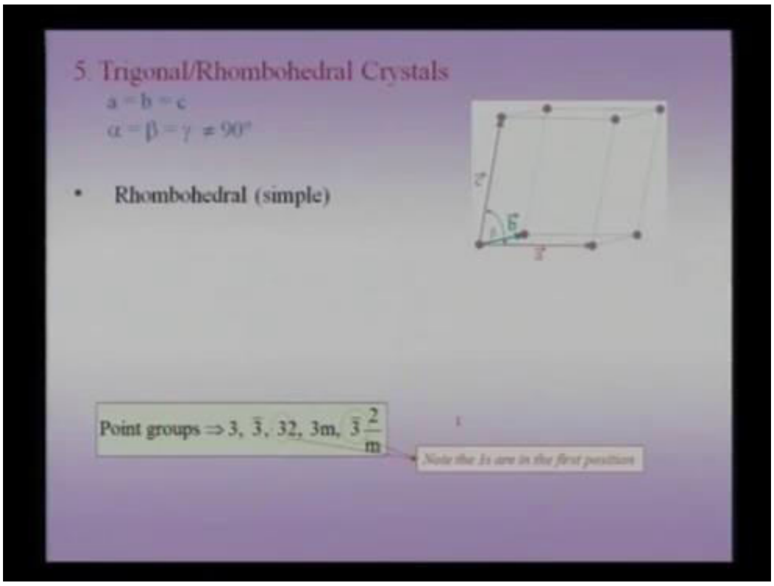

5. Trigonal/Rhombohedral Crystals

$a = b = c$

$\alpha = \beta = \gamma \neq 90°$

- Rhombohedral (simple)

Point groups ⇒ 3, $\bar{3}$, 32, 3m, $\bar{3}\frac{2}{m}$

Note the 3s are in the first position

So, in trigonal crystals and we already seen how we can go from a unit cell of a cubic to the trigonal unit cell, by pulling along the body diagonal. And if we do a such an operation we land up with a is equal to b equal to c alpha, beta, gamma all equal, but not equal to 90 degrees. That means, this angles can be any general angle, in this case also we have only one kind of lattice, the simple rhombohedra lattice and all rhombohedra crystals are characterized by the 3 fold or a 3 bar axis of course, a 3 in the first position.

We had noted earlier that the cubic crystals the way they are written, are characterized by 2 3 folds, and the 3 occurs in the second place in the point groups. In the case of trigonal crystals and rhombo hedral being the synonym of trigonal, we note that the three is in the first place. So, all rhombohedra lattices and some crystals based on them would have 3 bar 2 by m symmetry with the 3 in the first place, and rhombo hedral crystals could have a lower symmetry, and these symmetry include 3 m, 32, 3 bar and 3.

So, this is an important distinction to be noted, whenever the point is written, and we note that the 3 is in the first place, then we have to be sure that it is a trigonal crystal. And whenever the 3 is in the second place it refers to a cubic crystal and not a trigonal crystal, additionally in the trigonal crystals there is one and only one 3 fold axis, why in cubic crystals they at least have 2 3 fold axis, which automatically results in 4 3 fold axis, so that has to be kept in mind. In differentiating the cubic crystals from the trigonal crystals.

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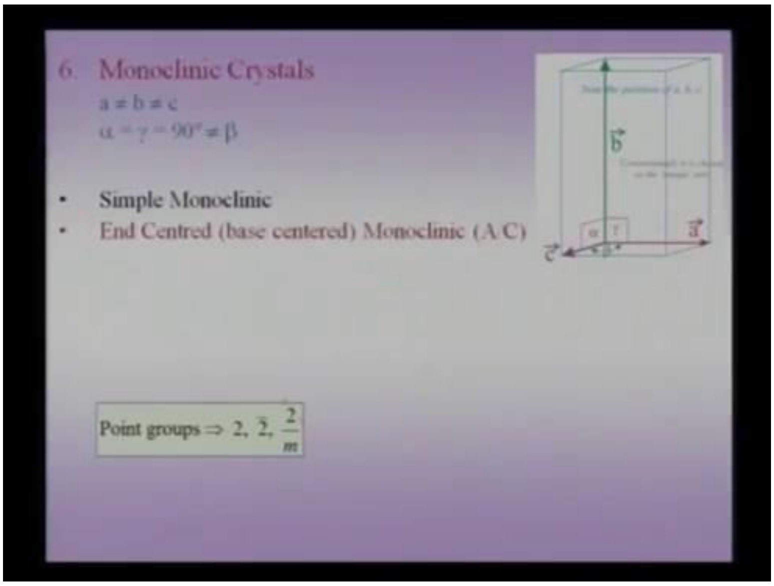

6. Monoclinic Crystals

$a \neq b \neq c$

$\alpha = \gamma = 90° \neq \beta$

- Simple Monoclinic
- End Centred (base centered) Monoclinic (A/C)

Point groups $\Rightarrow 2, \bar{2}, \frac{2}{m}$

If you go down lower in symmetry we have the monoclinic crystals, and we already seen that the monoclinic crystals can be based on 2 kinds of monoclinic lattices, the simple monoclinic. And the end centred which is sometimes called the base centred the monoclinic lattice, this centring could be the A or C centring in other words the centring could be opposite the a vector or opposite the c vector. So, we could have two kinds of centring for the n centred lattice.

And therefore, crystals based on this monoclinic crystals could have that centring, and the symmetry of monoclinic lattices is always at least has the symmetry 2 by m. While crystals based on monoclinic lattice could have 2 by m, 2 bar or a 2 kind of a point group symmetry. We can clearly see that as a good down the list the symmetry of the crystals is lowered, and we will soon classify them on a decreasing order of symmetry in a one of the coming slides.

STUDENT: Excuse me sir why do you have written the order of you has written is specific.

Mr Ravi, has a important question that the I have written these point groups in a certain order or way is this any specific order to it, I do not remember the way in which I wrote order. But, the most specific way of the bright way of writing is by increasing order of the point group, so each point group is defined by the number of identity point at least, in other words how may of the independents symmetry operations it has got. And if you count those number of symmetry operations, which would be called the order of the point group. The most preferred way of writing these point groups is by an increasing order of the point groups that is the way of writing it correctly.

STUDENT: Actually as you have told that three is in the first position. So, which is they are always there in the first position or it can be changed.

You are asking two independent questions, so Mr Ravi specific question is that regarding the portion at 3 and in this case the question is of the 2 perhaps. We are asking 2 independent questions, are these point groups in the way they are written are they written in a particular sequence, which is a logical sequence. The point number 2 if of course, within a to differentiate one kind of the crystal from the other, when you differentiate one kind of crystal from the other.

Then you worry about the position of 3 or the position of 2 or the number of these kinds of 2 by m, for instance of orthorhombic crystals, we had seen that it has 2 by m, 2 by m, 2 by m. In other words all the primary axis are having 2 by m symmetry 2 fold an a mirror perpendicular to it. But, this monoclinic crystals have just one kind of such kind of 2 by m symmetry along one of the axis, which is happens to be the preferred axis b typically.

Now, further I am telling that the logical way of ordering these point groups apart from the of course, highest symmetry one, which is the symmetry of the what you may call the polyhedral class, is also to the order it in terms of increasing order of the point group, which I am not sure I have done here.

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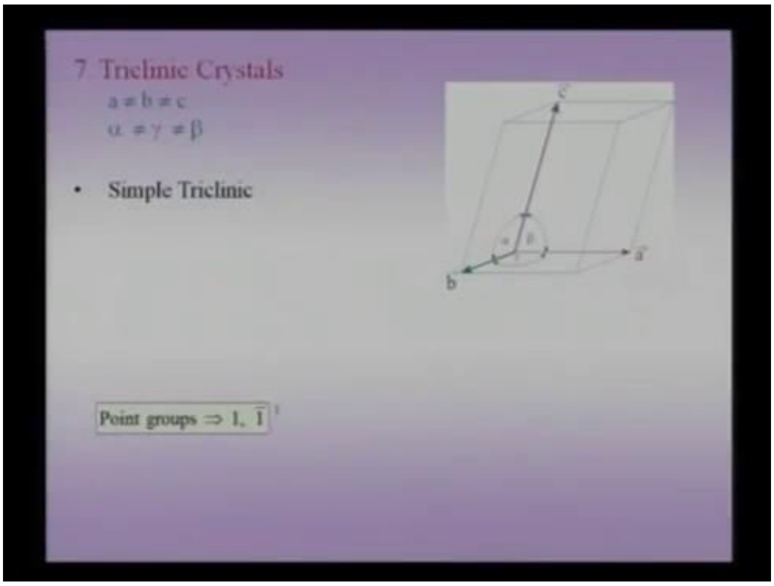

7 Triclinic Crystals

$a \neq b \neq c$

$\alpha \neq \gamma \neq \beta$

- Simple Triclinic

Point groups ⇒ 1, $\bar{1}$

So, when we get pointed out that the lower symmetry one is a triclinic crystal, and a triclinic crystal for instance has no special symmetry, the highest symmetry you can think of is a centre of inversion, which is the 1 bar kind of a symmetry. And triclinic crystals are basically characterized by the translation of symmetry and of course, if 1 bar is present we all, so side that kind of symmetry. And we had noticed that for the triclinic crystals, they are always based on the triclinic single simple triclinic lattice, and there is no special relationship a among the lattice parameter for a triclinic crystal.

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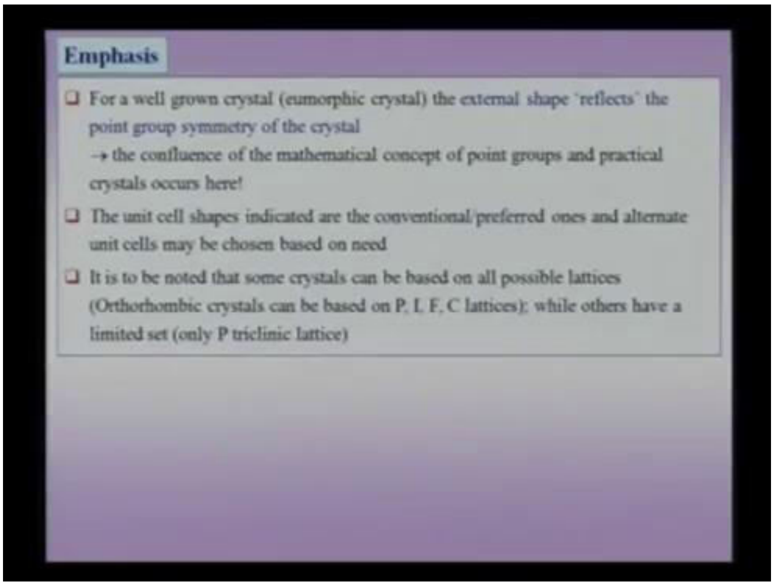

Emphasis

- ☐ For a well grown crystal (eumorphic crystal) the external shape 'reflects' the point group symmetry of the crystal
  → the confluence of the mathematical concept of point groups and practical crystals occurs here!
- ☐ The unit cell shapes indicated are the conventional/preferred ones and alternate unit cells may be chosen based on need
- ☐ It is to be noted that some crystals can be based on all possible lattices (Orthorhombic crystals can be based on P, I, F, C lattices); while others have a limited set (only P triclinic lattice)

So, we have slowly gone through the 7 crystal systems, we have briefly outlined symmetry and the preferred unit cell and the lattices which belong to this 7 crystal systems. And we are more importantly noted, when we especially discussed the cubic crystal is a connection between the shape of the crystal, and the internal symmetry present in the crystal. And this is what written in the first sentence here, the external shape reflects the point group symmetry of the crystals.

And this is the confluence of the mathematical concept of point groups, and the practical concept of shape of crystals. And we have already noted the unit cells can be chosen according to our need at the point of time, but they are always preferred units cell which we conventionally choose. And we also notice that all kind of lattices may be present or it may just be based on primitive kind of lattice.

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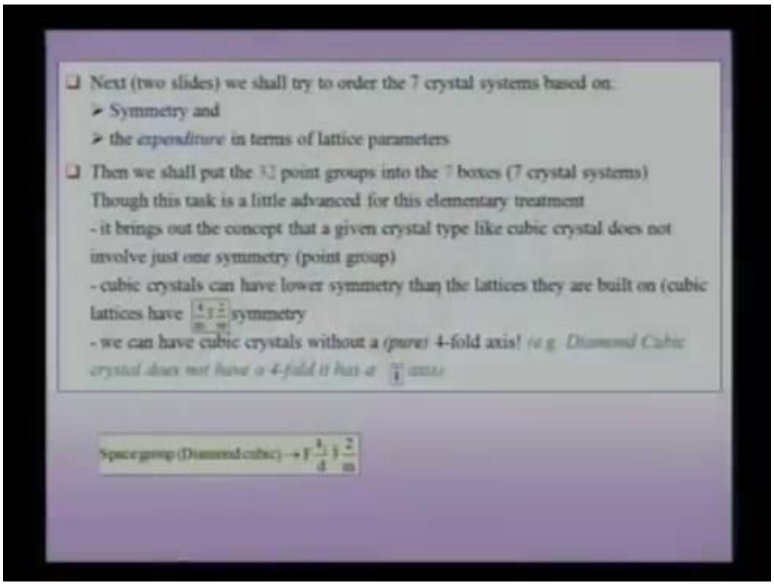

- ❑ Next (two slides) we shall try to order the 7 crystal systems based on:
  - ➢ Symmetry and
  - ➢ the *expenditure* in terms of lattice parameters
- ❑ Then we shall put the 32 point groups into the 7 boxes (7 crystal systems)
  Though this task is a little advanced for this elementary treatment
  - it brings out the concept that a given crystal type like cubic crystal does not involve just one symmetry (point group)
  - cubic crystals can have lower symmetry than the lattices they are built on (cubic lattices have $\frac{4}{m}\bar{3}\frac{2}{m}$ symmetry
  - we can have cubic crystals without a *(pure)* 4-fold axis! *(e.g. Diamond Cubic crystal does not have a 4-fold it has a $\bar{4}$ axis)*

Space group (Diamond cubic) → F $\frac{4_1}{d}\bar{3}\frac{2}{m}$

Next we will try to order these 7 crystal systems, the ones we have considered, so far based on symmetry and expenditure in terms of lattice parameters. And essentially what we are doing, we are taking a 32 point groups and putting them into 7 boxes, these 7 crystal systems. And we have already noted that for instance the cubic crystals can have a lower symmetry, than the lattices they are built on.

For instance, we note that some are the cubic crystals may not have a pure 4 fold axis, for instance is a diamond cubic crystal is written with a space group F 4 by 1 d 3 bar 2 by 2. In other words it is characterized by 4 1 screw axis, and if you are just looking at the point group symmetry we can also think of it having a 4 bar kind of an axis. So, we will now try to classify this 7 crystal systems based on symmetry, and also based on the expenditure of the lattice parameters.

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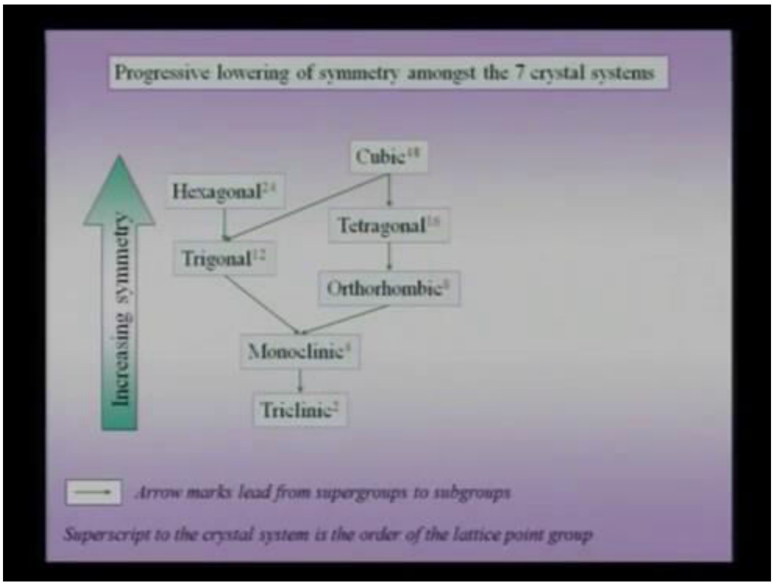

Progressive lowering of symmetry amongst the 7 crystal systems

Increasing symmetry

Cubic^{48}

Hexagonal^{24}

Tetragonal^{16}

Trigonal^{12}

Orthorhombic^{8}

Monoclinic^{4}

Triclinic^{2}

Arrow marks lead from supergroups to subgroups

Superscript to the crystal system is the order of the lattice point group

First based on symmetry we already seen the lower symmetry one is the triclinic crystal, and the higher symmetry one is the cubic crystal. Now, the way this ordering is done is that we locate the order of the point group, in other words if we take the cubic crystal then we try to see that the hodrohydral cubic crystal, as how many independent symmetry operations right. So, in other words if I start with the single point, after this point group as operated I would like to locate all the equivalent points, which is the point group as generated.

So, in the case of cubic crystals 48 such points would be generated and therefore, it got the highest symmetry, this tree apart from listing these various crystal systems, in terms of an increasing order of symmetry also sort of by these arrow marks, points out to be sub groups. A sub groups is concept, where in we try to understand if the symmetries are contained with another symmetry, for instance we already noted that if you take a simple example of the 6 fold axis. Then we know a 3 fold or a 2 fold axis is contained within the 6 fold axis.

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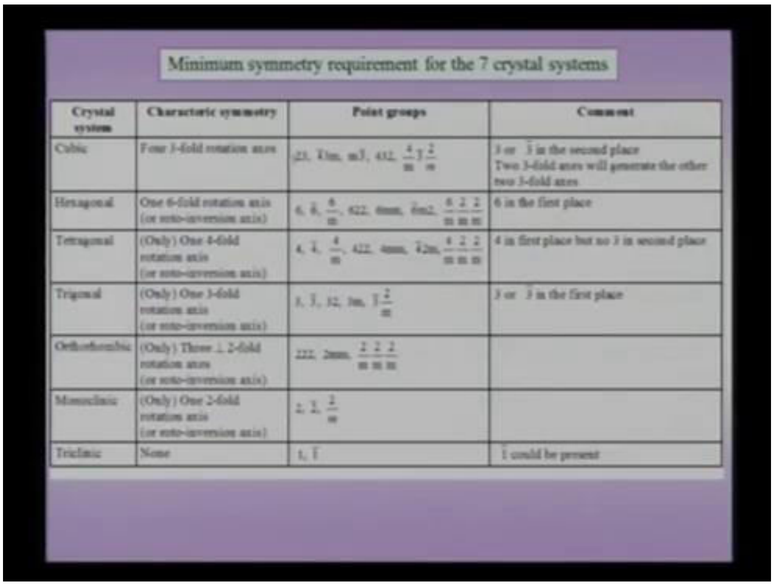

Minimum symmetry requirement for the 7 crystal systems

Crystal system	Characteristic symmetry	Point groups	Comment
Cubic	Four 3-fold rotation axes	23, $\bar{4}3m$, $m\bar{3}$, 432, $\frac{4}{m}\bar{3}\frac{2}{m}$	3 or $\bar{3}$ in the second place Two 3-fold axes will generate the other two 3-fold axes
Hexagonal	One 6-fold rotation axis (or roto-inversion axis)	6, $\bar{6}$, $\frac{6}{m}$, 622, 6mm, $\bar{6}m2$, $\frac{6}{m}\frac{2}{m}\frac{2}{m}$	6 in the first place
Tetragonal	(Only) One 4-fold rotation axis (or roto-inversion axis)	4, $\bar{4}$, $\frac{4}{m}$, 422, 4mm, $\bar{4}2m$, $\frac{4}{m}\frac{2}{m}\frac{2}{m}$	4 in first place but no 3 in second place
Trigonal	(Only) One 3-fold rotation axis (or roto-inversion axis)	3, $\bar{3}$, 32, 3m, $\bar{3}\frac{2}{m}$	3 or $\bar{3}$ in the first place
Orthorhombic	(Only) Three ⊥ 2-fold rotation axes (or roto-inversion axis)	222, 2mm, $\frac{2}{m}\frac{2}{m}\frac{2}{m}$	
Monoclinic	(Only) One 2-fold rotation axis (or roto-inversion axis)	2, $\bar{2}$, $\frac{2}{m}$	
Triclinic	None	1, $\bar{1}$	$\bar{1}$ could be present

Similarly, let us go down and may be pick up let me say some work we take a slide here, for suppose we take a cubic crystal 4 by m 3 bar 2 by m, we see that the 2 3 symmetry is contained within these 4 by m 3 bar 2 by m.

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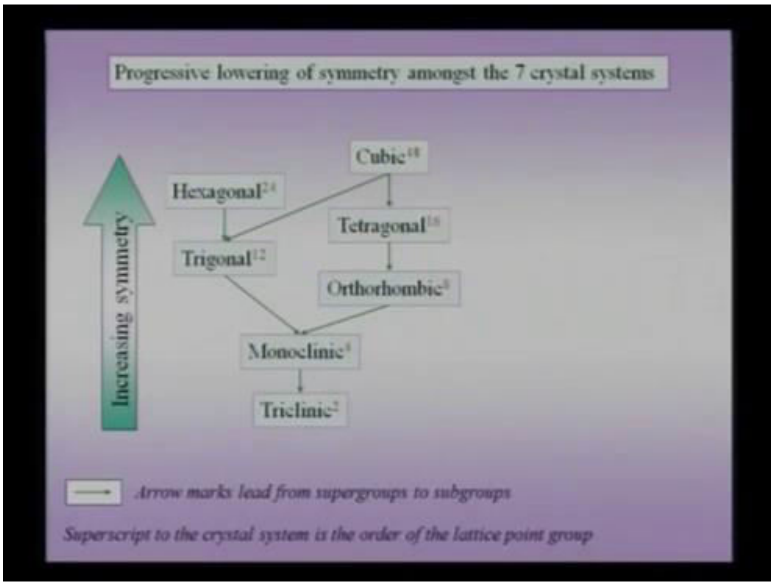

Progressive lowering of symmetry amongst the 7 crystal systems

Arrow marks lead from supergroups to subgroups

Superscript to the crystal system is the order of the lattice point group

In other words it is a sub group of the crystal, so how do we rank this in terms the order of the point groups, and order of the operators, which lead to the point group. The cubic is the highest, which has the order 48, hexagonal has an order 24, but we have to note that the hexagonal is characterized by a 6 fold, a cubic is characterized by 2 3 folds, and they are not sub groups of each other. Then the tetragonal is characterized by 16 operations or order 16, trigonal order 12, orthorhombic order 8, monoclinic order 4 and triclinic order 2.

The subgroup relations should be cubic the orthorhombic is the sub group of the tetragonal, which is subgroup of the cubic. And if I track from the bottom, the triclinic is the subgroup of the monoclinic, which is subgroup of the orthorhombic, which is subgroup of the tetragonal, which is subgroup of the cubic. So, I have an unbroken chain of sub group starting from the cubic and leading to the triclinic, I can use an alternate chain, alternate path to go to cubic the triclinic is subgroup of the monoclinic crystals.

The monoclinic is the subgroup of the trigonal and the trigonal is the subgroup of the cubic. Another way of going to the top or to the hexagonal crystal would be the third path the triclinic is the subgroup of the monoclinic, which is the sub group of the trigonal, which is the subgroup of the hexagonal crystals. So, we can clearly see from this diagram that some of the crystals have higher symmetry than the other crystals, and the way we rank those symmetries is based on the order of point group. So, we have the lowest symmetry once in the bottom, and the higher symmetry once at the top. And we can by this network identify the groups and subgroups, and this is an important concept especially later on when we deal with properties, and other kind of concepts which are related to crystals Mr Patel has the question.

STUDENT: Sir I have a simple question, if I consider benzene, a benzene planar crystal and there are the 6 fold axis, and what is the centre of inverse sir. So, if we write the total symmetry groups we obtain one group just to you have written here, so suppose you describe all the crystal structures. So, you can draw any one example and, so how we can see the all points.

Very good question, so there are 2 important issues which you have raised, one is the symmetry of the for instance an isolated tree like benzene tree. So, the question Mr, Patel has got is that suppose I am dealing with the benzene tree, and it is an isolated molecule for instance, the symmetry of that then of course, have a crystal based on that molecule. Now, these are 2 independent things we already seen, for instance you could have a very high symmetry molecule or a low symmetry molecule.

But, then when you make a crystal out of that, then this is an independent concept all together right, we have seen that for instances you could even have the cubic lattice. But, then if you place a low symmetry molecule in it, and that performs a role of the motif then it could have a low symmetry crystal. Now, this very concept you were mentioning we actually discussed in detail in the chapter one symmetry, but here we are talking about order of the point group.

So, we are not talking about the independent entities which go on to make the crystal system. And we are taking the highest point group of the whole hedral class that is what we are considering here, we already seen within a cubic class itself there are many lower symmetry crystals also which have a lower order right. So, we are considering the highest order one in making this classifications, so that point has to be absolutely clear.

Regarding individual benzene rings at this point of time I would not mix myself at this concept, ultimately I will have a crystal, I will find out I will assume for now that the crystal has got the highest point group. And I am trying to then classify those in an increasing order of symmetry, but this individual molecule and understanding that symmetry of those molecule is a e task, which we took up in the chapter on symmetry.

So, that is a independent task and that would not bother as now because, you could start with for instance an hexagonal benzene ring and land up with a crystal I do not know what the crystal structure benzene would form. But, it could form a crystal structure which is lower in symmetry, than the hexagonal symmetry which it for instance could have for instance.

STUDENT: Sir, that will depend on how we pack the molecule.

Absolutely, so how we pack the molecules, and for now I will try to pack take those molecules, which will give me the crystal of the highest symmetry. Because, we are given writing a point order of the operation as 48; that means, that I am using the hodrohydral class for this classification.

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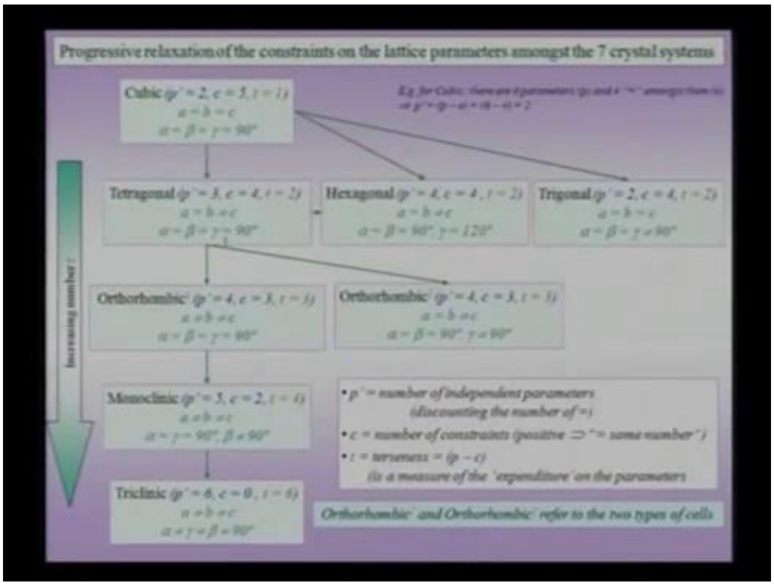

Progressive relaxation of the constraints on the lattice parameters amongst the 7 crystal systems

Cubic ($p' = 2$, $c = 5$, $t = 1$)
$a = b = c$
$\alpha = \beta = \gamma = 90°$

Tetragonal ($p' = 3$, $c = 4$, $t = 2$)
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

Hexagonal ($p' = 4$, $c = 4$, $t = 2$)
$a = b \neq c$
$\alpha = \beta = 90°, \gamma = 120°$

Trigonal ($p' = 2$, $c = 4$, $t = 2$)
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

Orthorhombic' ($p' = 4$, $c = 3$, $t = 3$)
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

Orthorhombic'' ($p' = 4$, $c = 3$, $t = 3$)
$a = b \neq c$
$\alpha = \beta = 90°, \gamma \neq 90°$

Monoclinic ($p' = 5$, $c = 2$, $t = 4$)
$a \neq b \neq c$
$\alpha = \gamma = 90°, \beta \neq 90°$

Triclinic ($p' = 6$, $c = 0$, $t = 6$)
$a \neq b \neq c$
$\alpha \neq \gamma \neq \beta \neq 90°$

- p' = number of independent parameters (discounting the number of =)
- c = number of constraints (positive ⊃ "= some number")
- t = terseness = $(p - c)$ (is a measure of the 'expenditure' on the parameters

Orthorhombic' and Orthorhombic'' refer to the two types of cells

This is the task now, the previous one was the purely symmetry based argument now this is purely an expenditure on the lattice parameters. So, this is in some sense a lesser important task, but just for a what you might call an understanding of the unit cells, and the preferred lattice parameters for those unit cells, we want to understand how they rank in terms of the and we had done this exercise for the two dimensional crystals.

And we had seen that we defined a parameter known as terseness which is nothing, but the number of for instance, let me do a calculations for the cubic lays there are 6 parameters p, and there are 4 equal to among them. Therefore, my number of terseness value the p prime is p minus c which is 6 minus 4 which is 2, and the terseness which we have 5 constraints therefore, my terseness would be 6 minus 5 which is equal to 1. That means, if my expenditure on independent parameters is less, then higher is that kind of an unit cell in this hierarchy.

So, let me consider classify them, and let us start with cubic case and we saw that we have 5 constraints 1, 2, 3, 4, 5 equations. And therefore, these is 5 and therefore, we got an terseness value of 1, for the tetragonal one of these parameters is not equal to and therefore, we have 4 constraints, and my terseness value is 2. So, is it for the hexagonal class, where in now all the angles are constrained as before, but now one of the angles is different and we have a number of constraints is 4, the terseness value is 2.

And similarly for the tetragonal terseness value is 2 there are two constraints, the triclinic has the no constraints on the lattice parameters therefore, terseness value is 6. Now, what is table does for you is that when we looked at the previous table, we saw that there is the cubic, tetragonal, orthorhombic, monoclinic, triclinic, hierarchy, and that was based on symmetry. Now, based on our choice of unit cell, we have an different hyraces here from the cubic.

We can have the lower level, which is the next level which is the tetragonal hexagonal tetragonal. The next level would be orthorhombic then the mono clinic then the tri clinic, as you go down this tree, you will find that the terseness values that mean you are spending more on the lattice parameter, which is in some sense reflection of the fact that. Now, we are considering unit cell of a lower symmetry. And this is not the unit symmetry of the crystal, but the unit cell and therefore, we have to spent more on the lattice parameters. And therefore, the terseness values goes up and this goes down in the chain, so this is just a way of writing down the 7 crystal systems and the preferred unit cells.

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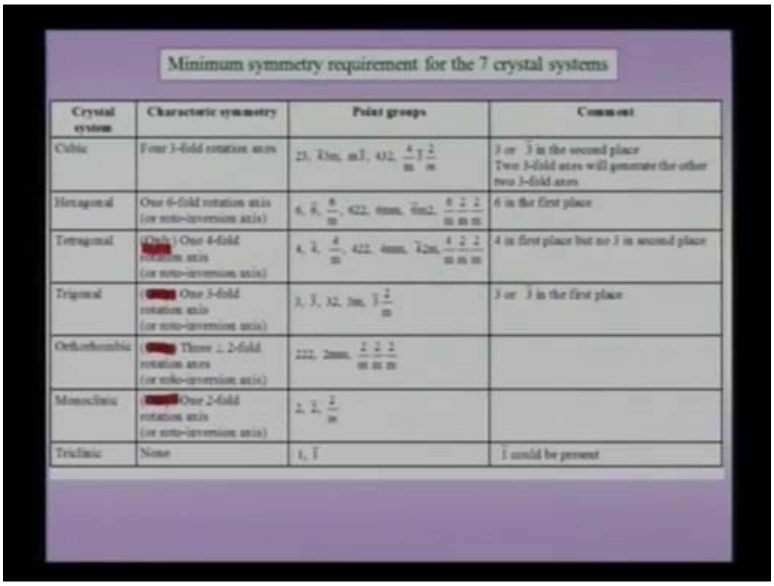

Minimum symmetry requirement for the 7 crystal systems

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Cubic	Four 3-fold rotation axes	23, $\bar{4}3m$, $m\bar{3}$, 432, $\frac{4}{m}\bar{3}\frac{2}{m}$	3 or $\bar{3}$ in the second place Two 3-fold axes will generate the other two 3-fold axes
Hexagonal	One 6-fold rotation axis (or roto-inversion axis)	6, $\bar{6}$, $\frac{6}{m}$, 622, 6mm, $\bar{6}m2$, $\frac{6}{m}\frac{2}{m}\frac{2}{m}$	6 in the first place
Tetragonal	(Only) One 4-fold [redacted] axis (or roto-inversion axis)	4, $\bar{4}$, $\frac{4}{m}$, 422, 4mm, $\bar{4}2m$, $\frac{4}{m}\frac{2}{m}\frac{2}{m}$	4 in first place but no 3 in second place
Trigonal	([redacted] One 3-fold rotation axis (or roto-inversion axis)	3, $\bar{3}$, 32, 3m, $\bar{3}\frac{2}{m}$	3 or $\bar{3}$ in the first place
Orthorhombic	([redacted] Three ⊥ 2-fold rotation axes (or roto-inversion axis)	222, 2mm, $\frac{2}{m}\frac{2}{m}\frac{2}{m}$	
Monoclinic	([redacted] One 2-fold rotation axis (or roto-inversion axis)	2, $\bar{2}$, $\frac{2}{m}$	
Triclinic	None	1, $\bar{1}$	$\bar{1}$ could be present

You already seen this, and now let us write down the full table, the full table indicating the 7 crystal systems. The characteristics symmetry the point groups in the crystal system and the comments regarding this kind of a symmetry, and we had already seen for instance that the hexagonal crystal for instance is characterize by 1 6 fold rotation axis, and this is written in a way, so basic in the first place. So, we made, so now, we understand the complete picture of the crystal system, the characterizing symmetry all the point group which are contain within the crystal system.

And how to identify them based on a simple rule system for instance, suppose I want to identify diagonal crystal I would to try like for 3 or a 3 bar in the first place. So, if c or a 3 or a 3 bar in the first place in a point group, then I can clearly see this is a trigonal crystal. And an important comment we had made while discussing try clinic crystal is that, the triclinic crystals would have a 1 bar symmetry which means it can have a centre of inversion of course, triclinic crystal could also have low symmetry, which is otherwise written as an 1 fold symmetry.

So, this is an important summary of all the 7 crystal system and there point groups, and once in for all we have clearly set that crystal system are based on symmetry, and not the geometry of the unit cell. So, this point has to be absolutely clear I will leave this slide little bit for you, so that you can see this and observe all the information and in this slide, and try to use it in useful wave whenever are you see point group of any crystal. And the important words to be noted are the words only wherever they appear, so you see that you have used the word only in many contacts that have to be noted.

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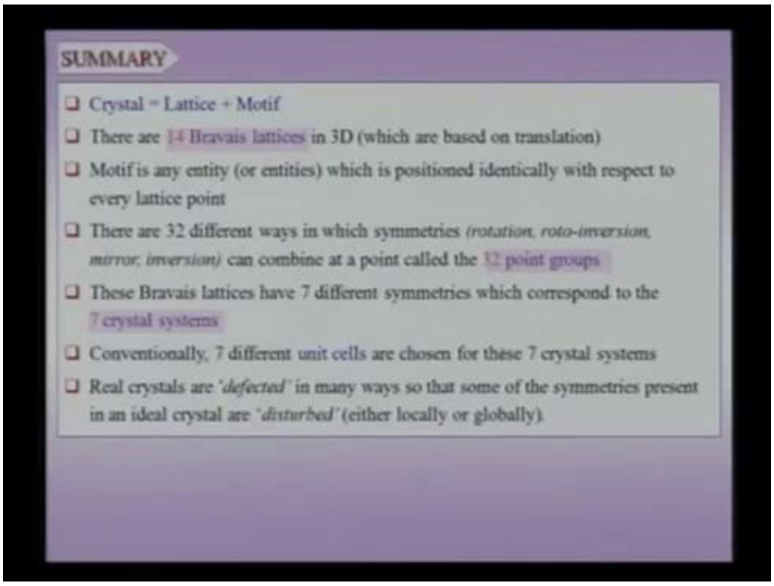

SUMMARY

- ☐ Crystal = Lattice + Motif
- ☐ There are 14 Bravais lattices in 3D (which are based on translation)
- ☐ Motif is any entity (or entities) which is positioned identically with respect to every lattice point
- ☐ There are 32 different ways in which symmetries *(rotation, roto-inversion, mirror, inversion)* can combine at a point called the 32 point groups
- ☐ These Bravais lattices have 7 different symmetries which correspond to the 7 crystal systems
- ☐ Conventionally, 7 different unit cells are chosen for these 7 crystal systems
- ☐ Real crystals are '*defected*' in many ways so that some of the symmetries present in an ideal crystal are '*disturbed*' (either locally or globally).

So, it is time to summarize, the silent features we have learned, so far, so they are as follows as listed in this. A crystal is a lattice plus motif, there are 14 bravais lattices in

3D, which are based on translation, a motif is any entity which is position identically with respect to every lattice point. We will have a few more question to ask regarding in one of coming slides, there are 32 different ways in which symmetries can combine, and this lead us to the 32 point groups.

This bravais lattices have a 7 different lattices symmetries, which correspond to the 7 crystals systems. Conventionally there are 7 unit cell which are chosen for the 7 crystal systems, real crystals this is an important point and we will have a lot to say about this, real crystal are defected in many ways. So, that some other symmetries present in a ideal crystal are disturbed, and this disturbances could be locally or globally so in other words real crystal could be very different from the ideal mathematical crystal we have just know constructed.

And we will of course, try to understand how they are different from the ideal crystals we have constructed. So, just to highlight the important point the 14 bravais lattices the 32 point group, the 7 crystals systems and of course, you not tell it in detail there is another numbers which come up which is the 230 space groups.

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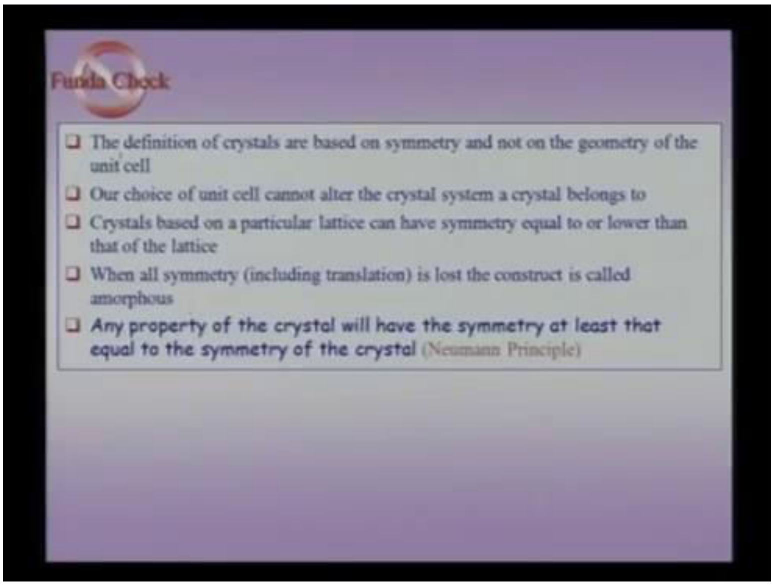

Funda Check

- ❑ The definition of crystals are based on symmetry and not on the geometry of the unit cell
- ❑ Our choice of unit cell cannot alter the crystal system a crystal belongs to
- ❑ Crystals based on a particular lattice can have symmetry equal to or lower than that of the lattice
- ❑ When all symmetry (including translation) is lost the construct is called amorphous
- ❑ **Any property of the crystal will have the symmetry at least that equal to the symmetry of the crystal** (Neumann Principle)

So, let us check what you learn, so far and I just read this slide for you the definition of crystals based on symmetry, and not the geometry of the unit cell. Our choice of unit cell cannot alter the crystal a system crystal belongs to, crystals based on a particular lattice can have a symmetry equal to that or lower than that of the lattice. When all symmetry including translation lost, the construction the I mean entity we have made is called amorphous.

And in very important thing which we consider any property of the crystal will have at least the symmetry equal to symmetry of the crystal or typically could be even higher than the symmetry of the crystal. And when we talking about symmetry, we talking about the point group symmetry in this contest, and this is the principle known as the Neumann principle. So, all the language symmetries and all crystal trophy can be directly co related with the properties and specially symmetry of the properties.

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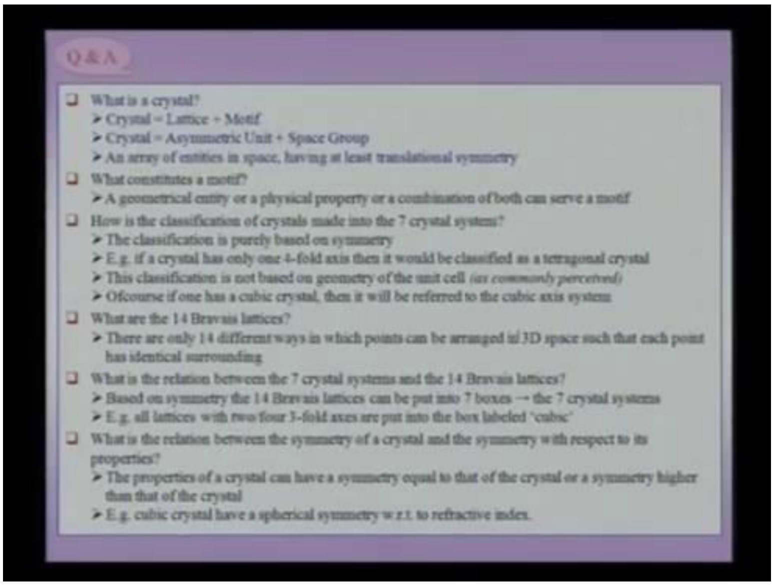

Q & A

- ❑ What is a crystal?
  - ➢ Crystal = Lattice + Motif
  - ➢ Crystal = Asymmetric Unit + Space Group
  - ➢ An array of entities in space, having at least translational symmetry
- ❑ What constitutes a motif?
  - ➢ A geometrical entity or a physical property or a combination of both can serve a motif
- ❑ How is the classification of crystals made into the 7 crystal systems?
  - ➢ The classification is purely based on symmetry
  - ➢ E.g. if a crystal has only one 4-fold axis then it would be classified as a tetragonal crystal
  - ➢ This classification is not based on geometry of the unit cell *(as commonly perceived)*
  - ➢ Ofcourse if one has a cubic crystal, then it will be referred to the cubic axis system
- ❑ What are the 14 Bravais lattices?
  - ➢ There are only 14 different ways in which points can be arranged in 3D space such that each point has identical surrounding
- ❑ What is the relation between the 7 crystal systems and the 14 Bravais lattices?
  - ➢ Based on symmetry the 14 Bravais lattices can be put into 7 boxes → the 7 crystal systems
  - ➢ E.g. all lattices with two four 3-fold axes are put into the box labeled 'cubic'
- ❑ What is the relation between the symmetry of a crystal and the symmetry with respect to its properties?
  - ➢ The properties of a crystal can have a symmetry equal to that of the crystal or a symmetry higher than that of the crystal
  - ➢ E.g. cubic crystal have a spherical symmetry w.r.t. to refractive index.

So, let us now answer a few question we have learned, so far and the akriti I will help me with this answering this question. So, let me ask the first questions what is a crystal.

STUDENT: Crystal equal to lattice plus motif, crystal equal to a symmetry unit plus space group. And area of entities in space having at least translations symmetry.

What constitutes amounts of motif.

STUDENT: A geometrical entity or physical property or a combination of both can serve a motif.

How is a classification of crystal made into the 7 crystal system.

STUDENT: The classifications is fairly based on symmetry example, if a crystal is n only one 4 fold axis, and it would be classified as a tetrahedron crystal. This classification is not based on geometry of the unit cell as commonly perceived of course, if one has the cubic crystal then it will be refer to the cubic axis system.

What are the 14 bravais lattices.

STUDENT: There are only 14 different ways in which point can be arrange in 3D space, such that each point has identical surrounding.

What is the relationship between the 7 crystal system and 14 bravais lattices.

STUDENT: Based on symmetry the 14 bravais lattices can be put into 7 boxes, the 7 crystals system. Example, all lattices with 2 fold, 3 fold axis are put in to the box labelled cubic.

What is the relation between the symmetry of the crystal the symmetry with respect to it is properties.

STUDENT: The properties of crystal can have a symmetry equal to that of the crystal or symmetry had in that of the crystal. Example, cubic crystal have a spherical symmetry with respect to reflective index.

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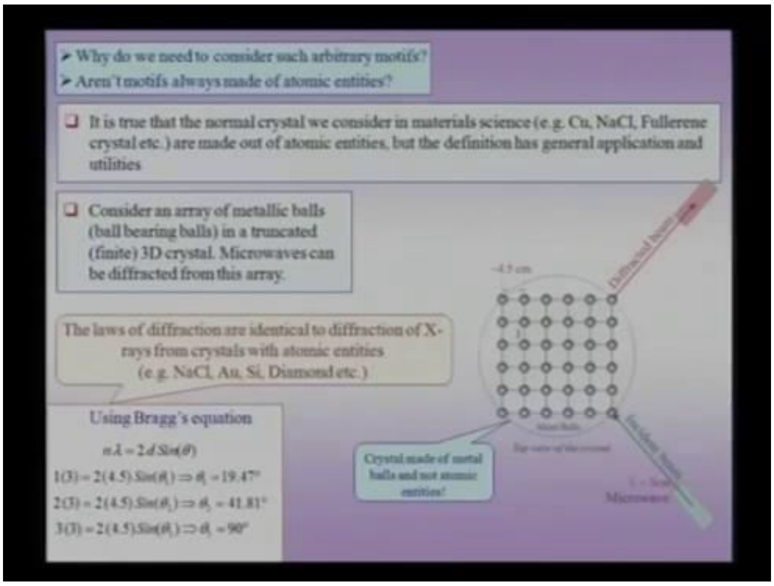

- Why do we need to consider such arbitrary motifs?
- Aren't motifs always made of atomic entities?

❑ It is true that the normal crystal we consider in materials science (e.g. Cu, NaCl, Fullerene crystal etc.) are made out of atomic entities, but the definition has general application and utilities

❑ Consider an array of metallic balls (ball bearing balls) in a truncated (finite) 3D crystal. Microwaves can be diffracted from this array.

The laws of diffraction are identical to diffraction of X-rays from crystals with atomic entities (e.g. NaCl, Au, Si, Diamond etc.)

Using Bragg's equation

$n\lambda = 2d\,Sin(\theta)$

$1(3) = 2(4.5)\,Sin(\theta_1) \Rightarrow \theta_1 = 19.47°$

$2(3) = 2(4.5)\,Sin(\theta_2) \Rightarrow \theta_2 = 41.81°$

$3(3) = 2(4.5)\,Sin(\theta_3) \Rightarrow \theta_3 = 90°$

Crystal made of metal balls and not atomic entities!

So, I will thank akriti for helping me out with the answers, next we consider another important question, why do we need to consider such arbitrary motifs. For instance, we have already consider very various kind of geometrical shapes in which we had arranged function triangular and more complicated shapes, and even chosen in very arbitrary kind of motif in the describe what motif are, so the question we are asking is that are in motif always made of atomics entities.

So, will try to understand this question by considering a crystal made out of typically this are the ball baring balls which going to a cycle for instance. Now, the question is that it is true that the normal crystal we consider material science for instance copper, sodium chloride, fluorine etcetera are made up atomic entities. But, the definition as general application and utilities, and the experiment I am going to describe now typically done in many Msc labs, Msc physics labs.

And the experiments is as follows that the ball baring crystal is constructed, actually you taken area of ball baring balls. So, they take put them in a array, and make a two dimensional crystal out of heat, then you uses pressure typically made of some kind of formed policy diary or a pole retie firm. And then top of that you make another array 2 dimensional array such box of in another words you can construct a three dimension crystal.

Now, the motif in this three dimensional crystal is an microscopic entity it is nothing, but a ball baring ball. So, the crystal which I make would look as the picture shown here, and this is just the projection from the top, and in this case what I can do I can do a diffractions experiment. And we know that for suppose if we look at the diffraction experiment, you would send X rays into material for instance a crystal of sodium chloride.

Here is a using X rays I would use microwaves, and typically the wave of such microwaves would be 3 centimetre, which is of the same order as this spacing of the ball baring balls. So, my wave length of the microwave is similar in to the lattice parameters spacing, and this is an importance requirement for diffraction to take place right. Whenever you do back diffraction once in the wave length of X rays is very similar to the lattice parameters spacing of the atomic crystal, and which is for instance sodium chloride from which bragged it is original experiment.

So, this crystal is now made of metal balls and not of atomic entities, and I can use my bragg's equation, which is m lambda equal to 2 d sin theta. And I can obtain various speaks at various positions for instance at 19.4 7 degrees, 41.81 degrees and 19 degrees. In other words, now I can make crystal made of ball baring balls, and I can actually do a diffraction experiment, in other words I send a beam of mono chromatic micro waves and get a diffractive beam, and various angles.

In other words, the lost of diffraction are identical to diffraction of X ray from crystals with atomic entities. For insane this diffraction experiment with the X rays I could do one sodium chloride, gold silicon or diamond, in other words the language of crystallography does not change, the loss of diffraction does not change, if I go from atomic entity crystal to crystal of this can which is microscopic crystal. Therefore, my languages needs to be constant across this lens scales, and later we will consider and I would like to point out people of made colloidal crystals.

In colloidal crystals, this are typically spheres, micron size sub micron size sphere which is go into form a crystals. And this crystals this sphere themselves Could be amphora’s for instance, and silica spheres are typically use make to some of this colloidal crystals. Therefore, the entities which go on to make a crystal could be in diversion scale there could be order arm strong, they could be of the microns, they could be the order of centimetres.

And they could perform experiment of diffraction, either with X rays with light or even micro wave and my results would be identical. As long as my geometry of the crystal and this scattering distance and the symmetry of the crystal is that, which is I use my language crystallography to describe. So, this is an important example we should note, that I need not constrain myself in the definition of a crystal, to only the atomic motifs because, the language is just applicable to border class of crystals as I pointed out, and there are been other example where they have crystallize viruses.

So, virus as you know can part time the living organism, but they can also crystallize and of course, in that state they are not active. But, you can perform a diffraction experiment from then, and they would perform a rule of a motif in that crystal, so this are examples with diverse examples and you know a single virus would constant of atomic entities.

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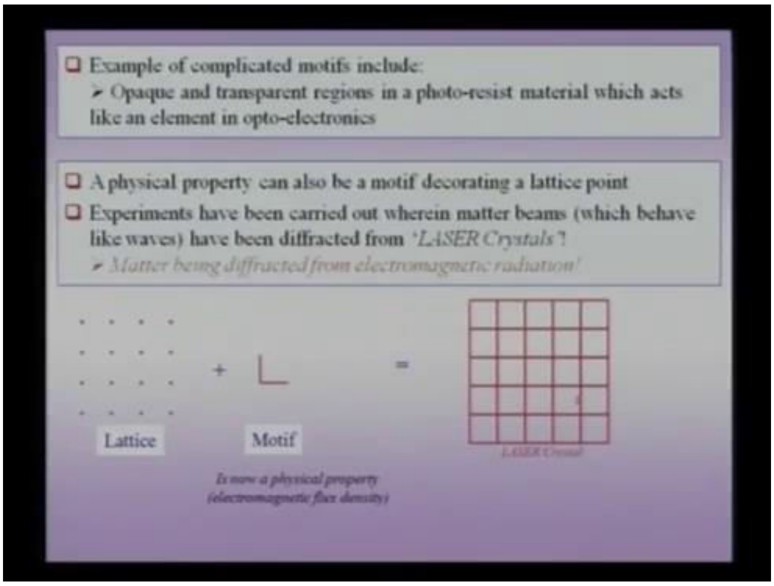

- ☐ Example of complicated motifs include:
  - ➢ Opaque and transparent regions in a photo-resist material which acts like an element in opto-electronics

- ☐ A physical property can also be a motif decorating a lattice point
- ☐ Experiments have been carried out wherein matter beams (which behave like waves) have been diffracted from *'LASER Crystals'*!
  - ➢ *Matter being diffracted from electromagnetic radiation!*

Another example for different kind of crystal would be they you could actually h, you could actually what you might call affect photo resist materials, with opaque and transparent reason, which can like in act like an element in opto electronics. Therefore, I can take a photo resist material, and then make an impression an optical impression which can act. And therefore, the motif in this case is nothing, but a reason which is opaque or transparent in a photo resist material.

And I can make a three dimensional crystal, if you like or a 2 dimension with this photo resist materials. And even more cures examples is the one which I am showing below and I was pointing out that of course, we may take up more examples later in the course that is physical property can also serve as a motif, which can go unto decorate a lattice point. So, experiments have been performed and especially this kind of experiments were perform the last 10 years within the last 10 years that is where in for instance I make a crystal.

And this crystal is now made up of purely laser beams; that means, this red line you see are laser beam. So, you have laser beam in 2 directions, so this 2 dimensionally laser crystal if you like to call it, and clearly if I make a square crystal out of you can see that this a laser crystal can be understood in our familiar language of crystallography by construing a square lattice and a motif in a shape of an L. Additionally alternately of course, I can choice an alternate motif which I will show on the board.

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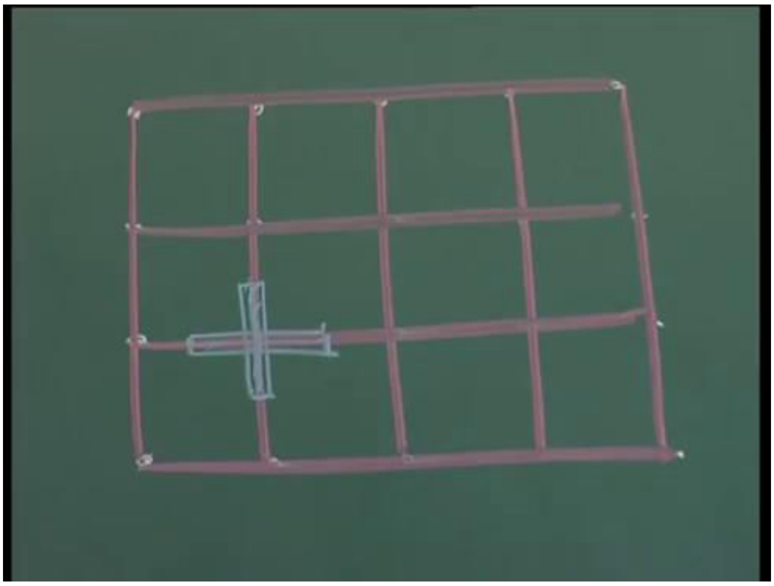

So, alternately I could construct motif which is in the form a plus, so each lattice point can be decorated a motif which is this part of the practice. So, each lattice point I put this plus which is nothing, but a intensity of light here, so in other word this is a very cure experiment, where in people have actually made a lattice or a crystal to be motto size, the crystal made out of laser beams and actually have diffracted matter through it.

So, this is an inverse of the what the common diffraction experiment which you might think of very new actually have a crystal made of atomic entities, and you would send an electromagnetic radiation to the diffract from here, from that kind of atomic entity. So, this is inverse of the problem, in this problem what I am doing I am making a crystal out of electromagnetic radiation which is laser crystal. And of course, this are red lines would indicate certain current of density in electromagnetic density.

And I can actually diffract matter out of this kind of a crystal, and this is possible because, you know matter can act according to braggs equation likewise. So, we can clearly see that there are crystal of divert types and, but for all this crystals we can use a common language a crystallography. And physics of this kind of crystals depending of course, a suppose for instance the physics we are talking about this the diffraction physics is a exactly identical as long as the common criteria for diffraction is made that is the wave length is similar to the spacing in the lattice of the spacing in the crystal.

So, we can have this kind of cures experiment and this kind of cures kind of motif which go on to the decorate lattices. So, in this lattice for instance they are no atomic entities and this is purely describe in terms of physical properties, which is now the electromagnetic radiation density.

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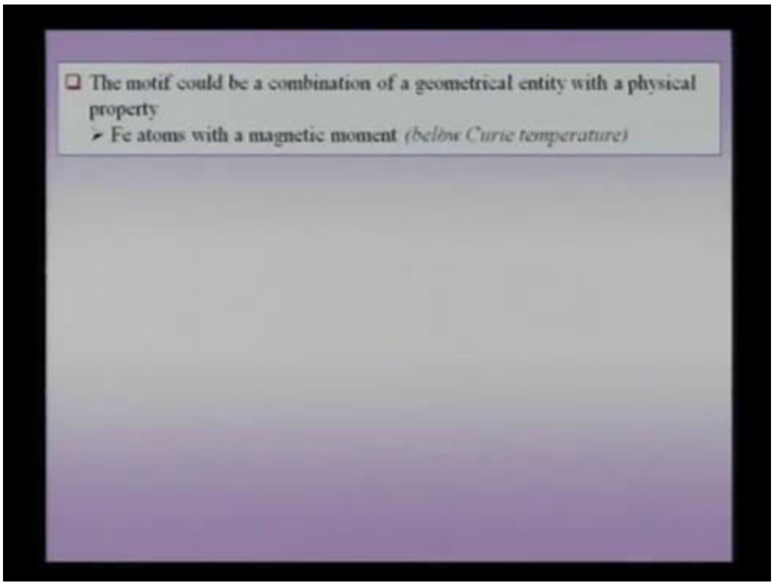

- ☐ The motif could be a combination of a geometrical entity with a physical property
  - ➢ Fe atoms with a magnetic moment *(below Curie temperature)*

So, we could have diverse kind of crystals and, but the language of crystallography remains the same, and the analyses in term of that languages also remains the same. And I had also pointed out that we could also have a case where in a motif could be combination of a geometrical entity and a physical property. For instance ions atoms with the magnetic moment, below the cure temperature would have of course, atomic position, in additional each atom would have magnetization vector which would typically within a dominion inside the material would be aligned.

So, now, I can describe the crystal in terms of just of course, the atomic positrons, but additionally I could take into account this magnetic moments. And I could describe this crystals of course, this is done with some addition to normal language of crystallography, and we use something known as a colour symmetry. And you have to note that this when we talk about the combination the symmetry of the structure could be lower.

Because, if all the magnetic moment are aliened then you would notice for instance even if I start with ions, which is the bcc ions the symmetry of the structure could be lower if all the magnetization vector are aliened. So, this is a case where in we need to consider a physical properties and the geometrical entity, you Mr, Ravi has a question.

STUDENT: Sir, in the case of Fe atom as well as the lattice magnitude moment below the temperature, while classifying the crystal we will consider both this properties simultaneously or we can take either or these the classify the crystal.

Very important questions, actually an a question which we are actually very soon going to other coming slides very next slide or another coming slide going to answer this question. So, the Mr, Ravi questions is that, when I am describing a Ferro magnetic ions, crystal of Ferro magnetic ion and I am sitting with in the domain of this Ferro magnetic ion. Now, that reason would I describe purely based on the symmetry of the ion atoms or should I take into account t magnetic moments.

As we shall soon see, they could do both this we could just ignore the magnetic moments and or we could take into accounts t magnetic moments. But, I will go to the board to explain you some possibilities.

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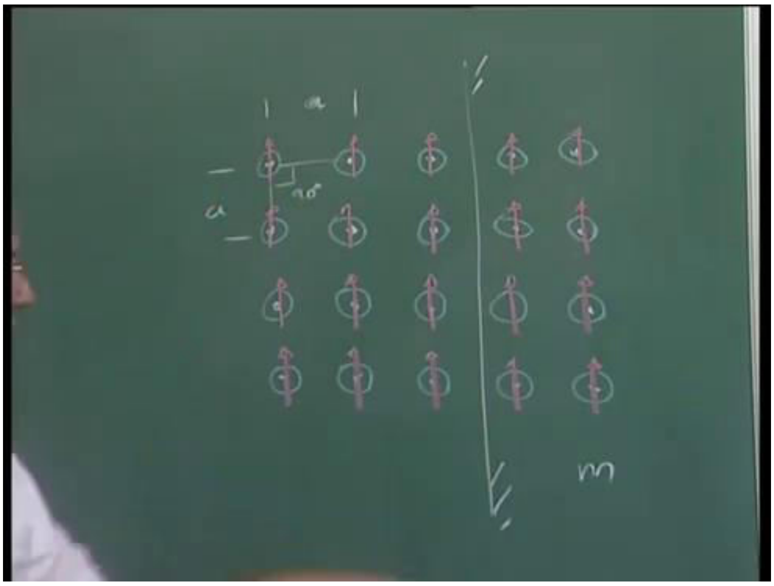

Now, let me constant ideal two dimensional crystal, now assume there are atomic entities sitting in this lattice positions, clearly the crystal had constructed now has got 4 mm symmetry and it is square crystal. But, now suppose I want to take it account the fact that suppose all them atoms are have in special moments which are a light, so in other word I am setting within a domain of the magnetize crystal.

Now, they are 2 possibilities when all this spins or the magnetic moment skied aligned, there is possibility that it can actually change the lattice parameter. But, to the original lattice parameter a and a this included angle was 90 degrees right, so my 2 lattice parameters of this same, and include 90 degree there for if this is square crystal. Clearly, now if I want to include the magnitude moments in my description of the crystal, this is no longer a square crystal.

Because, now the only symmetry present in this crystal the diagonal mirror would be lost the 4 fold axis would be lost. And therefore, I would have a plane here and this would have a lower symmetry and this would be a rectangle crystals, so this part we already know. But, important question I am asking which is what is relevant to your question is that, can this magnetization moment itself change the lattice parameters in addition to the fact that if I look at the symmetry it is already we know it is the rectangular crystal it could, so happen.

Because of the magnetization movement, there could be selective change in the lattice parameter. For instants either there could be expansion along this direction or one of those things can happen because, now the physical property is aligned, so there is no random, there is no average. And if that happens even the lattice parameter would change, and in that case automatically my 4 fold axis would be lost, and it could be the crystals of lower symmetry.

Even though I am not taking into account this magnetization vector in my description of the crystal, if the crystal lattice parameter changes as a consequence of this kind of an alignment. Then I can no longer call it higher crystal higher symmetry crystals, but automatically symmetry has been lower, assuming that, that kind of distortion is very small and it can be ignored, then when I ignore the magnetization movement I call it has square crystals anyway take into account the magnetization moment I will call it a rectangle crystal.

We had consider on our early stages of this lecture series, and advance definition of crystal which said crystal is equal to space group and symmetric unit. In the lattice plus motif definition, the lattice was performing the role how the reputation should take place, and the motif is what the entity which was to be repeated at lattice points.

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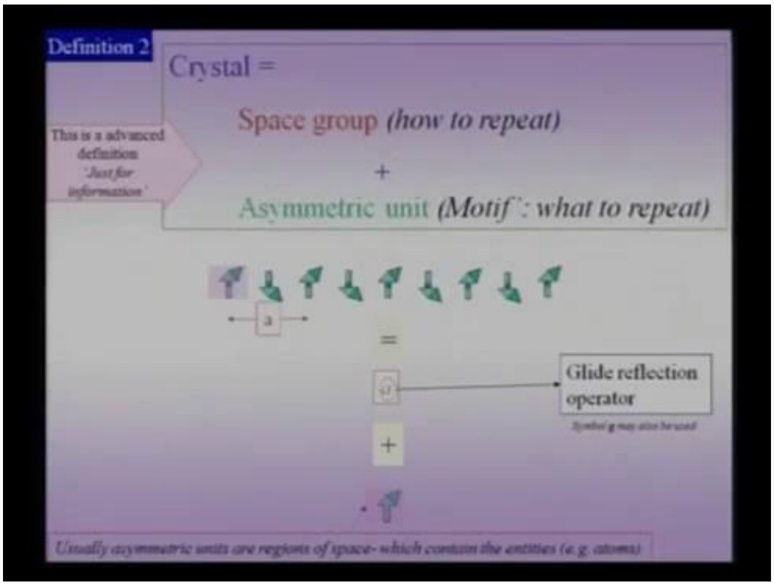

Definition 2

This is a advanced definition 'Just for information'

Crystal =

Space group *(how to repeat)*

+

Asymmetric unit *(Motif': what to repeat)*

Usually asymmetric units are regions of space- which contain the entities (e.g. atoms)

We have just said that this advance definition based on space group plus in the symmetric unit, which is typically the preferred in the language of crystallography is possible. Though we are not taking up this definition in detail in this course, I thought it be worthwhile that we consider one example of how such a description is possible. Now, let us consider an array of the arrow mark of course, this are decorated arrow marks with the certain kind of a triangle on top of the arrow marks.

Now, and you can see that the arrow mark have been inverted from point to point, so in a array of point initially, which had spacing a by 2 the first point I put an arrow mark upwards, and second point downwards and, so forth. Now, I can describe such a crystal which is now a one dimensional crystal decorated with a two dimensional motif, in other word I made the relaxation with respect to the dimensionality of the motif, which we did earlier repeatedly previous in various example to clarify certain concepts.

And, now I want to understand it in the language of space group and symmetric unit, now I can see that if I take this arrow mark it is repeated h at distance a. So, I could use this as lattice translation vector, and I could use it typically motif to describe it, but I will not do that I will use this more defined definition of the crystals. And in this case, now my space group operator would be glide reflection operator g is used as the symbol for it sometimes.

And what is the glide reflection operator do, suppose I have a repeat unit of a, the glide reflection operator moves a symmetric unit by distance a by 2 and inverse it, it moves it by a by 2 and inverse it, moves it by a by 2 and inverse it. So, we have seen that this is the property of the glide reflection operator, in other word suppose this is my pen which is the arrow mark with a certain decoration. It would move by a by 2 which is half of the lattice parameter and inverse, it will move it by a by 2 and invert it, it will move by a by 2 and inverse it and I will get the entire crystals.

So, now, I am considering a symmetry operator a glide reflection operator, and we have already seen the glide reflection operator has translation symmetry built into this operator along with this property of reflection. So, in other words the mirror plane for which is not a true mirror plane, but a glide reflection mirror plane, the horizontal plane can act like the mirror plane. So, the glide reflection operator is the more suffocated operator, and it operates on dissymmetric unit.

And as symmetric unit are typically region of space, so the region of space is marked by this pink colour box, and it contains the entity which is part of the motif, the original motif in the language of lattice plus motif. So, this pink region is taken mode over by a by 2 and inverted and therefore, whatever the contains of that unit are also moved and inverted.

So, therefore, I can write down this whole crystals as this asymmetric unit, which extends from say for a instants from here, which is from this is a by 2, this is a by 4 is minus a by 2 plus a by 4 and this is my extends, and with the certain zee extends or the other axis and with this space group operator which is g. So, in one dimension my g operator combine with this asymmetry unit would give me a crystal.

So, this is just perhaps and very simple and introductory way of introducing the concept of space group and asymmetric unit. But, this language is a language which is typically found in the international table of crystallography, and other region were they want to describe crystals. But, for now most of the concept we are dealing with or in the language of lattice plus motif.

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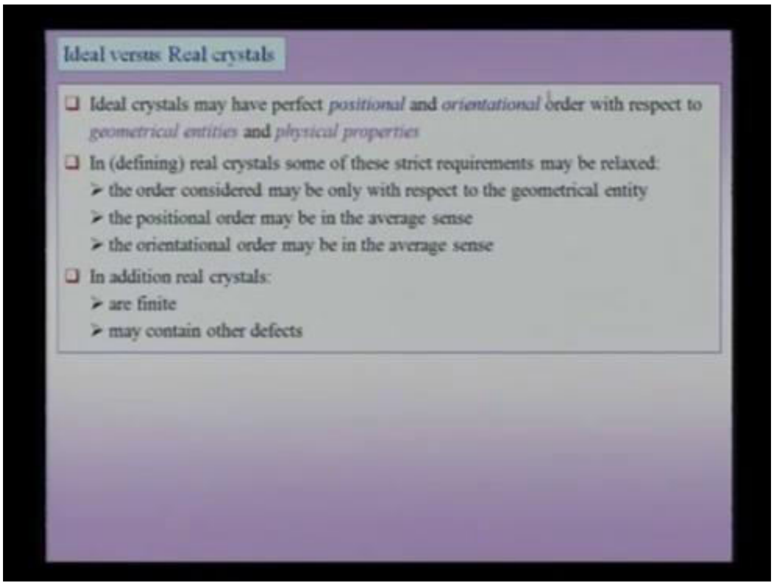

Ideal versus Real crystals

- ❑ Ideal crystals may have perfect *positional* and *orientational* order with respect to *geometrical entities* and *physical properties*
- ❑ In (defining) real crystals some of these strict requirements may be relaxed:
  - ➢ the order considered may be only with respect to the geometrical entity
  - ➢ the positional order may be in the average sense
  - ➢ the orientational order may be in the average sense
- ❑ In addition real crystals:
  - ➢ are finite
  - ➢ may contain other defects

So, let us return to the important question, the question which Mr, Ravi asked how do we go from ideal crystal, and ideal mathematical crystal, and reach a real crystal. So, something we met for note ideal crystals may have perfect positional or orientational order with respect to geometrical entities, and physical properties. In defining real crystal some of this strict requirements may we relaxed, so may relax some of this requirement, and we will do that in the form of flow chart in the coming slide.

So, we may only consider the symmetry or the order with respect to the geometrical entity, and we will also see later on that the positional order may be only in the average sense, and also the orientational order may be only in the average sense. In addition we note of course, that real crystals are finite and have other kind of defect.

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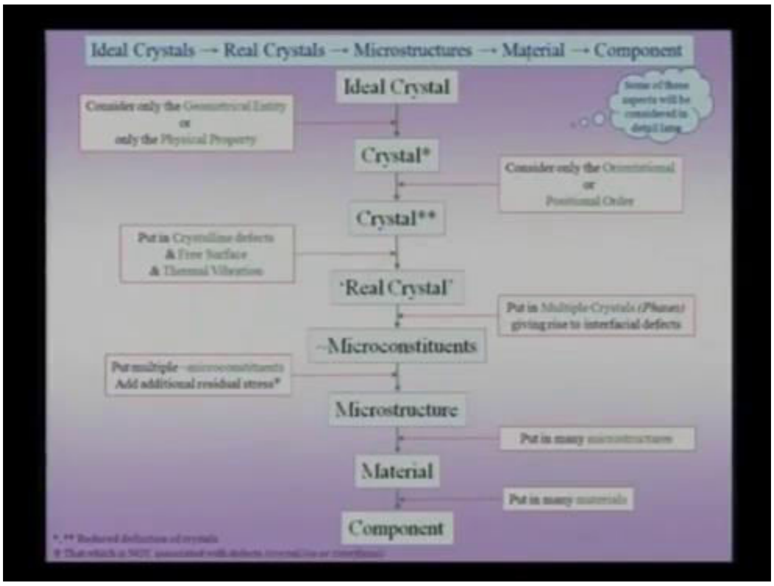

Ideal Crystals → Real Crystals → Microstructures → Material → Component

Ideal Crystal

Consider only the Geometrical Entity
or
only the Physical Property

Crystal*

Consider only the Orientational
or
Positional Order

Crystal**

Put in Crystalline defects
& Free Surface
& Thermal Vibration

'Real Crystal'

Put in Multiple Crystals (Phases)
giving rise to interfacial defects

~Microconstituents

Put multiple ~microconstituents
Add additional residual stress‡

Microstructure

Put in many microstructures

Material

Put in many materials

Component

Some of these aspects will be considered in detail later

*, ** Reduced definition of crystals

So, let us go from ideal crystals and in this case I have made the little future lead for extension of the logic, were in not only I am starting with ideal crystals I go up to an entire component. So, we know that all this entities the motif typically could be atomic scale, so we could typically talking about hand storms, and we are talking about other component which could be macro scale component, which would be centimetre or meters in dimension.

And we want to see how I can go from this ideal crystal and component and of course, at this state we will not consider all the concepts in detail, but we just want to outline a complete flow of the logic. So, that we can understand tomorrow that if suppose I have a failure in my component, then what are the length scale I need to consider the length scales are clearly across various dimension. So, you can have hang storms which is 10 power minus 10 meters to meters.

So, you may have to travel 10 orders of magnitude in terms of the dimensional space to in order to understand why the component at fail. So, there could be reasons in component level like for incense component could have sharp corner, which could lead to stress concentration. It could be at lower scale, it could be the scale which we call as we will see later what we will call the micro structure or it could be at even lower scale, and we need to consider all this scale, when we want to track down the problem.

So, let us see how we can go from ideal crystal to a real crystal to something known as micro structure of course, microstructure will be dealt with lot of detail the later part of the course. Then to a material which is what commonly dealing with for instant I have got the material with me which is of course, not a single material, it is the combination of wood certain kind of fibre which used as the duster, it could be material as chalk for instance, it could be any kind of the material.

And some of this are the example I am showing here are not crystalline, but here since we are doing mostly a description of crystals. And, so we will consider a example as if we are starting with real crystals, so let me start this long journey with an ideal crystal, and I will do this in two slide this slide and the next slide both. So, that this concept sink in slowly and some of the terminology additionally they are introducing here, also sinks in, but as I pointed out that some of this would only become clear much later in the course some of the terminology will understood in detail only later.

So, we have an ideal crystal now what I can do, I can only consider the geometrical entity or the physical property like we did in the case of the magnetization vector. So, I could do that and I could have a reduced definition of a crystal; that means, now the crystals is not is either consider in terms of the of physical property or the geometrical entity I do not want to consider both. Future I could even reduce the definition even future, by considering only the orientational or the positional order.

Now, for instance I could have a system which has both kind of an order, an orientational order and positional order, and I want to consider only one of the two in describing my crystal. At this stage of course it may be difficult for you understand all the implication of the statement, and we will take up examples later on to understand, what I mean by only orientational order or positional order. A simple example I will take one dimensional example to show you on the board, what I mean by the statement, but some more example will come up later.

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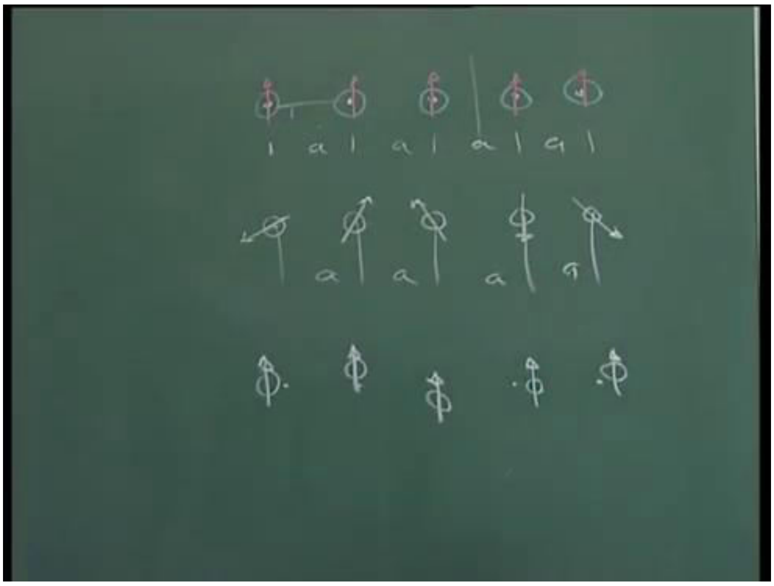

So, let me take one dimensional crystals here which I have drawn on the board were in I have the system which is perfectly orientational possibly order; that means, this distance is perfectly a as I go from each atom to the next atom right. Now, I could do something that now, so this system can be disordered with respect to the orientation functions and I go from one arrow to the next arrow. So, even though the spacing between the atoms is a the orientational order is not a maintain.

And therefore, I could have a reduce definition of the crystals in which I consider only the position order. The other possibility would be that there is positional disorder, but there is orientational order, in other word suppose this original lattice point which are a spaces I could put my atoms of course, I can do in one dimensions or two dimensions in various places with respect to the lattice point.

But, I put all my arrows in upward direction, so such a system is orientationaly order, but not positional order such a system on the top is positional order, but not orientationaly order. And I can use at the reduced definition of a crystal in which I consider only one of this kind of orders. And you will see better examples later on.

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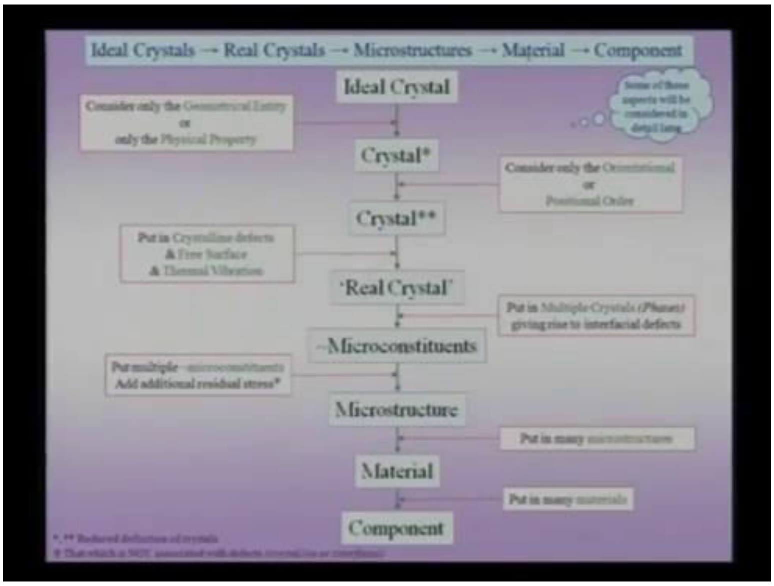

Ideal Crystals → Real Crystals → Microstructures → Material → Component

Ideal Crystal

Consider only the Geometrical Entity
or
only the Physical Property

Some of these aspects will be considered in detail later

Crystal*

Consider only the Orientational
or
Positional Order

Crystal**

Put in Crystalline defects
& Free Surface
& Thermal Vibration

'Real Crystal'

Put in Multiple Crystals (Phases)
giving rise to interfacial defects

~Microconstituents

Put multiple ~microconstituents
Add additional residual stress#

Microstructure

Put in many microstructures

Material

Put in many materials

Component

*, ** Reduced definition of crystals

Therefore, I could reduce my definition first by considering only the geometric entity of the physical property, and future reduces the definition based on orientational or positional order. Then I can go from still what you might call reduces definition of the crystals to oriel crystals were in I introduced crystalline effects.

And we will have the entire chapter devoted to the crystalline effects and we also need to note that we always have the finite crystals, we never have the infinite crystal in reality therefore, we have to introduce free surface. And the third thing which is thermal vibrations, and if I take a snap shot of an crystal at any point of time, the picture would look like the one I have shown here; that means, atoms are vibrating about their mean position, but they are displaced with respect to their atomic position, which I consider the seat of the lattice point.

Now, therefore, there are unavoidable defects in materials like crystalline defects free surface thermal vibrations. And therefore, I could have a real crystal which have these kind of defects, then it is not necessary that my entire material is made up of single kind of the crystals. I can put multiple crystals, which I call multiple phases and therefore, when I put in multiple crystals I not only have a free surface.

But, also have an inter face between the 2 material, for instant suppose I want to make a crystal which I can suppose for, now I am assume the crystalline material, then I would have the interface between this two kind of the crystals. So, this something which would come unavoidal when unavoidable when you put in multiple faces, and this would give rise to the concept of the micro constitute. So, this concept we will take up later in the course, were in we will see names like for instances per light.

Per light is an micro constituent, which is made up of and alpha F e 3 c which is typically found in plane carbon steel. So, you can see those kind of micro constituents, and they are made up of multiple phases with interfacial interface and inter face itself is a defect. Then I can put in multiple micro constituents and additionally I can add residual status, typically as you will see later that residual stresses are unavoidable material and there are multiple sources of the residual stresses which we will also see.

So, I can take in micro constituent and add residual stresses and I can get something known as the micro structure. Now, this is a new way of defining micro structure this is not the classical definition form in many places, were in micro structure is defined as a structure seen at high magnification. So, this in new way of looking micro structure, but this is functional way of looking micro structure, were in you have micro constituent and residual stress add in.

We will also define this micro structure in a slightly different way in a or different way compared to this flow diagram in one of the coming slides. But, starting with the microstructure I can put in many micro structure to make a material, so material typically you might what you might consider a block of material, natural consider of many micro structures. Of course, you would have single micro structure, which would be a treveling or simple example of a many micro structure case.

And finally, I can put in many materials to make a component, so a single component for instance which you practically see in everyday life could have many, many kind of materials. And often this materials all need not only be crystallized a single component could have a plastic region, a region with metallic, which is the reason is ceramic, so forth. So, therefore, all this kind of a material can go to whether to make a component which is; obviously, performing some function.

And this component itself could be a part of the larger machinery and therefore, that the next scale you would talk about single component going on to make a larger machinery, which is performing some useful functions. So, I can start with the ideal crystal and going thought this flow chart by relaxing certain consideration and introducing certain new definition, I can go to a component.

And not only I am going down in terms of certain kinds of what you might call an ideal mathematic description, but also I am going across length scales. So, this additional point as to be noted, so let us look at the same slide, because there are, so many new concepts involved, in slightly different way as shown in the next slide, and I thank professor conj ash balny for making this slide for me.

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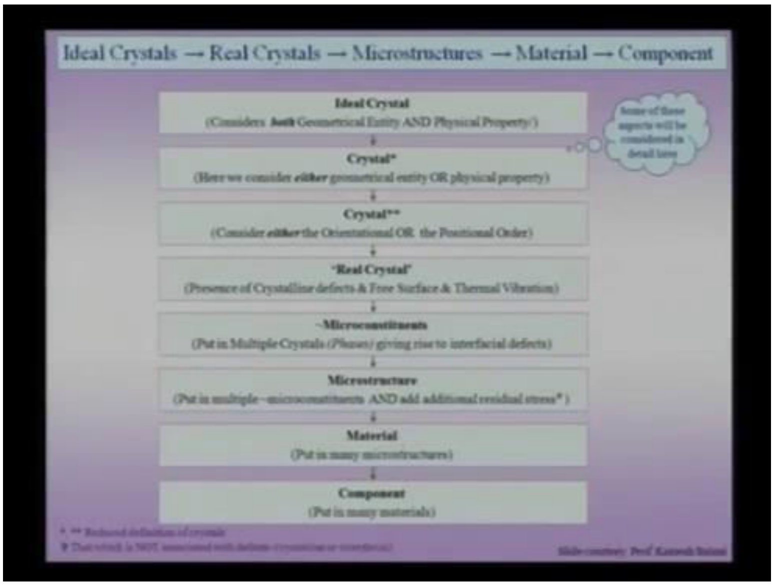

Ideal Crystals → Real Crystals → Microstructures → Material → Component

Ideal Crystal
(Considers *both* Geometrical Entity AND Physical Property)

Crystal*
(Here we consider *either* geometrical entity OR physical property)

Crystal**
(Consider *either* the Orientational OR the Positional Order)

"Real Crystal"
(Presence of Crystalline defects & Free Surface & Thermal Vibration)

~Microconstituents
(Put in Multiple Crystals (*Phases*) giving rise to interfacial defects)

Microstructure
(Put in multiple ~microconstituents AND add additional residual stress*)

Material
(Put in many microstructures)

Component
(Put in many materials)

Some of these aspects will be considered in detail later

*, ** Reduced definition of crystals

* That which is NOT associated with defects (crystalline or interfacial)

Slide courtesy: Prof Kantesh Balani

So, you have ideal crystals, real crystals, micro structure materials and components, so this an alternate way of representing the same thing. And, so we can have an ideal crystals which considers both geometrical entity and the physical property, I can have reduce definition of a crystal which I call a crystal star, were in I consider either the geometrical entity or the physical property. Further I could have even more reduced definition of a crystal, were in either I consider the orientation order or the positional order.

Future I could introduce various kind of defects, and we will consider this defect in detail later which are known as crystalline defects, I can reduce a free surface which is absolutely avoidable for any real crystal. And finally, thermal out vibration which is also unavoidable in real circumstances, then I can use this real crystal to actually construct what is known as micro constituent. Were in multiple crystals are put together and which will have any interface, which itself is a defect in the overall structure.

Finally, using this micro constituent I can construct a micro structure were in a multiple micro constituent and additionally I can put in some amount of the residual stress. And as we said, this kind of a definition micro structure is based on functionality because, this residual stress could have important application in a terms of the property of the material. Ultimately what I want to do in a real material is to have a micro structure property correlation or what we call more commonly, the structure property correlation.

And I want to understand this structure property correlation; obviously, I need to understand all the length scale below it, which means I need to understand the crystals, I need to understand the defect present in the crystal, and additionally this is residual stress. And therefore, this residual stress had been put into the definition of the micro structure therefore, the next stage would be to understand this micro structure property correlation, which is an important goal of material science.

Now, when you of course, I am looking at the component and the performance of the components especially in a bigger machinery were this component goes, I need to also look at the various accept regarding the mechanics of the component design of the component. Typically this is not under the basic per view material science, though we would also like to consider that, but as I said microstructure itself gives a important handle unto the property.

And therefore, I need to have the definition of the micro structure, and the understanding of the micro structure which of course, starts from various lens scale, and the first starting point would be an ideal crystal. So, I have the material in which are many micro structures and finally, I have a component which could be a combination of many, many materials.

And if you look at any working component in a modern machinery, you would note that it is made up of many, many materials if take a normal camera for instance, you would note that or a laptop or any one of this components or any one of the devices, which has components in it. You would note that many, many materials go on to make such a device, and it is very important for us to understand not only the individual constituent, but the assembly which finally, leads us to this grand component, and this grand machinery and the device.

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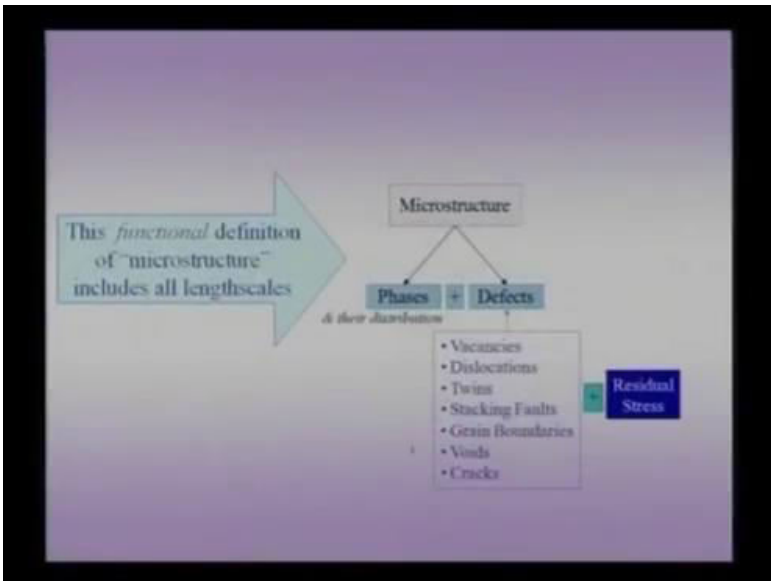

This *functional* definition of "microstructure" includes all lengthscales

Microstructure

Phases + Defects

& their distribution

- Vacancies
- Dislocations
- Twins
- Stacking Faults
- Grain Boundaries
- Voids
- Cracks

+ Residual Stress

So, we have seen that an important term which we have newly introduce in the sole structure is the micro structure. And this terms is very, very important from the material science perspective, and for instance in this course structure of material this is an important length scale. And if I understand my micro structure then quite a bit of my property could be understood based on this micro structure, and I am defining my micro structure slightly different here, which includes all my length scale.

So, what is the way I am defining my micro structure here, it is phases in the distribution, so I have multiple phases. And typically each one of this phase could be typically or enormous or it could be other kind of the phases, and I add defects to this distribution of phases. And these effect could be various kinds of crystalline defects like dislocation there could be larger defect, which are bigger in size for wades or crack some of the cracks should be big enough to seen with the naked eye. So, I put on all this effects in to the distribution of the phases and finally, add my residuals stress, which could give me at definition of a micro structure.

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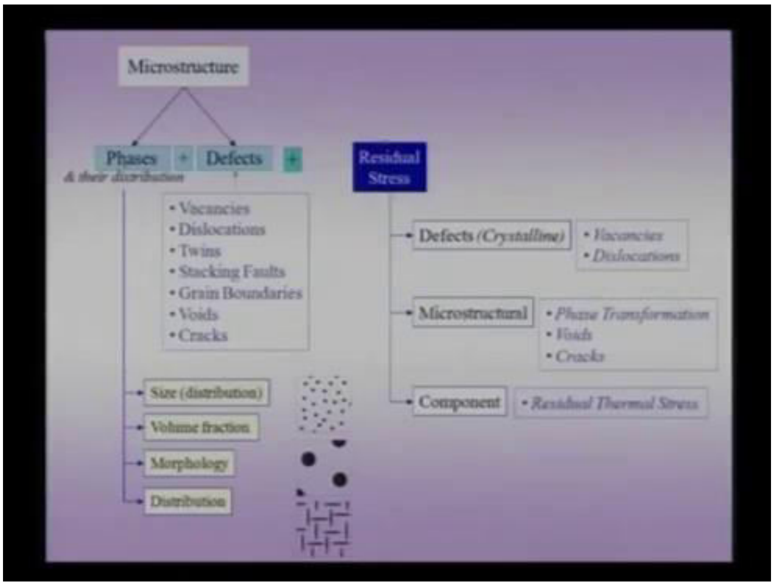

Microstructure

Phases + Defects +

& their distribution

- Vacancies
- Dislocations
- Twins
- Stacking Faults
- Grain Boundaries
- Voids
- Cracks

Size (distribution)

Volume fraction

Morphology

Distribution

Residual Stress

Defects *(Crystalline)*
- *Vacancies*
- *Dislocations*

Microstructural
- *Phase Transformation*
- *Voids*
- *Cracks*

Component
- *Residual Thermal Stress*

Now, the important point I need to consider is what do I mean when I mean phases in the distribution of course, will have lot to say about the defect structure in a material. And at this point I would like to describe little more about the very first thing in this the phases in the distribution, and also something about the origin of the residual stress. And this origin of the residual stress again like our journey into the component would involve multiple and length scales.

So, let me start with the origin of residual stress, the origin of the residual stress could be from very small length scale of the hand storm length scale, for instants defects in crystalline materials. They could be vacancies we will of course, what this is detail later, but there could be defects in the crystal function of vacancies are missing atoms in for instance for a copper crystal. There could be more complicated defects, line defect like dislocation whose extend of influence extends behind an atomic diameter.

There could be micro structure origin of residual stress for instance phase transformations or wide and cracks could led to residual stress. And of course, I am using iteratively the word micro structure within micro structure, but the way these definition are wide and cracks, we understand what is the origin of this kind of the residual stress. And finally, I could have thermal residual stress which are typically across the whole component.

And often you would notice that thermal residual stress can be used in the very beneficial way, for instance we can introduce surface compressive stresses which can tough in class. So, therefore, it is not necessary that residual stress always is bad it could be deleterious or it could be beneficial based on the situation, but residual stress is very, very important. And the behaviour of the material is quite a bit governed by the presence of this residual stress, and this is the reason that it has been included in the very definition of a micro structure in this course.

Now, look at look at phases and distribution, the word distribution hides with the net quite a bit of detail it may not be possible at this stage to go into all the details. But, take a small sampling of what you mean by phases and distribution for instant, what we could be talking about is a size and only a material may not have single size for instance suppose I am talking about a second phase, second kind of a crystal in the metric.

Then it may not be necessary that the second phase as the single size as I shown here, and it could have a distribution in sizes. But, I need to know the sizes, and size of all the particle which are present, and more important at statistical analyses of all the sizes which are called as size distribution. The second thing I need to know, when I am talking about phases and distribution is the volume fraction, in other words if it could be that this black phases with respect to the white matrix could be 10 percent in volume of fraction 20 percent in volume fraction or more.

And this would make a difference to a many properties therefore, I am talking about phases distribution I need to know the volume fraction or equivalently I may also want to know the weight fraction. Third thing I need to know the morphology of the phases, for instance suppose the second phase here is my black phase, it could be spherical or circular into two dimensional cross section or it could be in the shape of the needle has shown here. And this again would make the lot of difference to my properties, so is it circular or is it this needle shape would make a difference to my properties.

And finally, how this faces are distributed is also an important thing for instants here the size of the second phase is larger with respect to this, and assuming that the volume fraction is identical. Then this two distribution would have different properties when I am considering for instance a mechanical behaviour or anyone those kind of aspects, which would depend on my micro structure.

Now, this kind of a micro structure perhaps has the same volume fraction of this black phase, but now the distribution is change and this would again effect my properties. For instants additionally see that these needle shape thing have sharp corner, and this sharp corner could be a place where cracks could initiate. And therefore, my properties would change if I not only change my volume fraction, change my size and it is distribution, change the morphology of the crystal as you can see the morphology has changed.

That means, the shape of the crystal is change from here to here, and all this things put together would go on to describe a simple kind of the phase I use, which is phases and there distribution. So, let me try to once again emphases the important alternate way of defining a micro structure, which is perhaps more functional than we standard definition. In the standard definition we always define a micro structure as the structure seen at the higher magnifications, typically optical micro magnifications.

But of course, you could also have micro structure which are seen at in an transmission electron microscope, were in at your looking at nano structure. But, ignoring the scale aspect here and more emphasizing on the function aspect, we can call our micro structures as phases and there distribution. The defect structures within and these defect could be you defect within a single phases or between phases or could be more macroscopic like wide and cracks. And finally, we have to include residuals stress if we want to understand, the important thing which is known as the micro structure property correlation.

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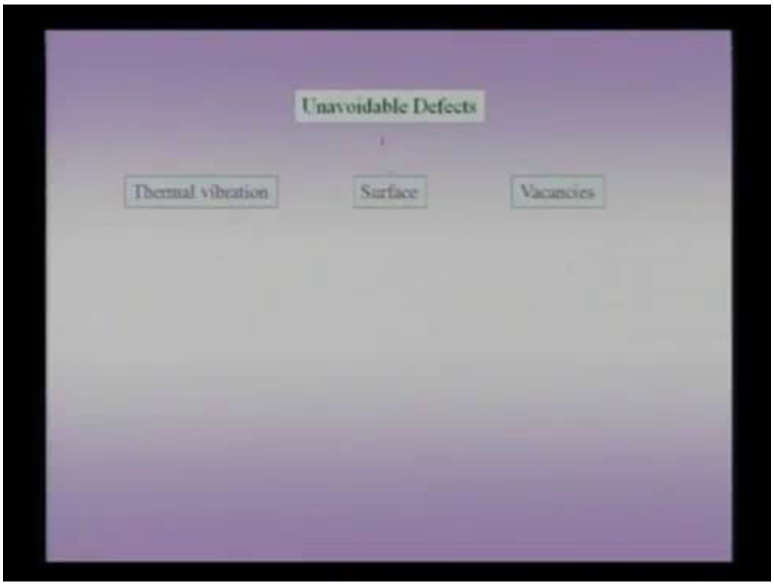

Unavoidable Defects

Thermal vibration

Surface

Vacancies

And emphases this important aspect that whenever I am talking about an ideal crystal versus real crystals, there are defect which are totally un avoidable how are ideally or how were nicely I like to prepare my material, try to make it a single phase material. And these three defect which always arise are thermal vibration, surface and vacancies, and this origin of vacancies get briefly touched upon, when we did try to understand what are the thermo dynamic quantities at the begging of this course. So, vacancies can be equilibrium thermo dynamic vacancies and therefore, they always arise at positive Kelvin temperatures. And these three defect always will be present in the crystal therefore, my crystal can never be an ideal mathematical crystal, and I have to work always with one of the reduce definition of a crystal.

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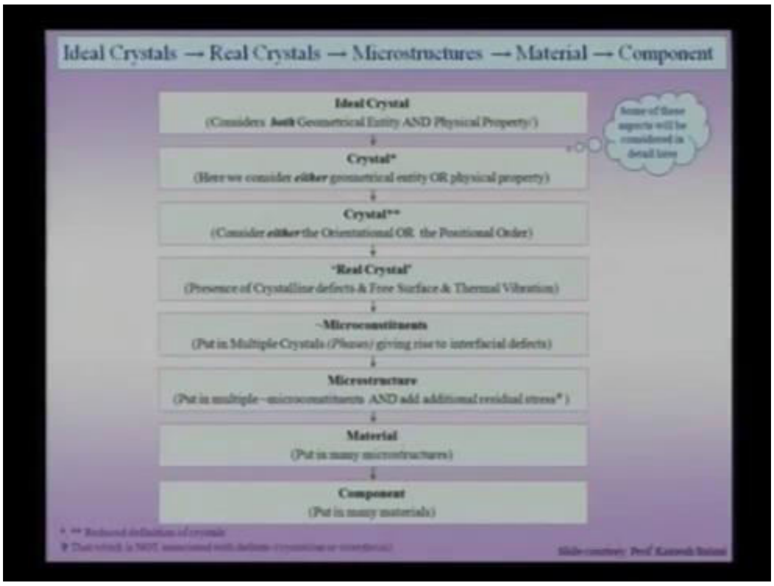

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(Put in many materials)

Some of these aspects will be considered in detail later

And more typically I would like starting from a ideal crystal move down to a more functional definition of micro structure. And the finally, the component were in now I am talking about a performance of the component, so I have the ideal crystal a properties of the micro structures. And finally, performance of a component, so this is our goal and at least till the micro structure we will take it up in this course on structures of materials.