Defects in Materials
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Lecture – 30
Twinning – 2

We have been talking or discussing about the twinning in material. We have considered initially both mechanical twin as well as the twin which can form during growth of crystals or during phase transformation.

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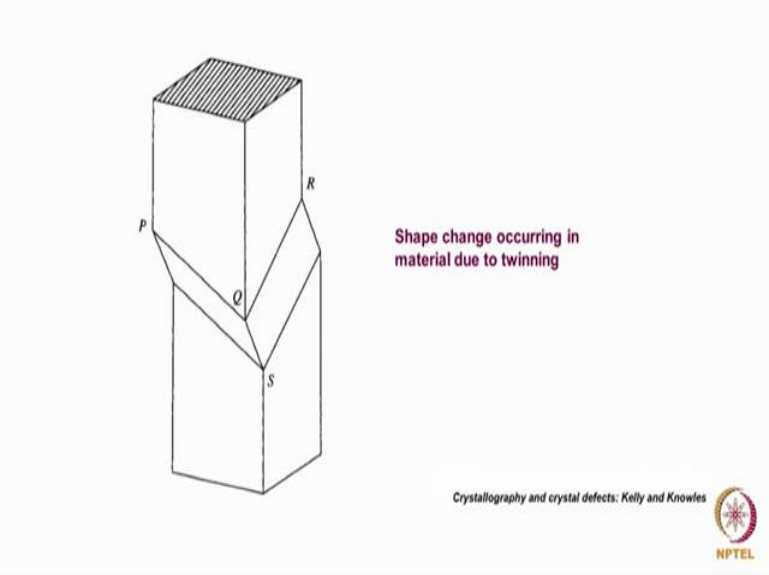

Mechanical twin essentially if you try to look at it whenever a twinning occurs as we can observe there is a deformation could be seen externally and the sample surface and we can observe that this is a homogeneous tilt of the external surface which is occurring.

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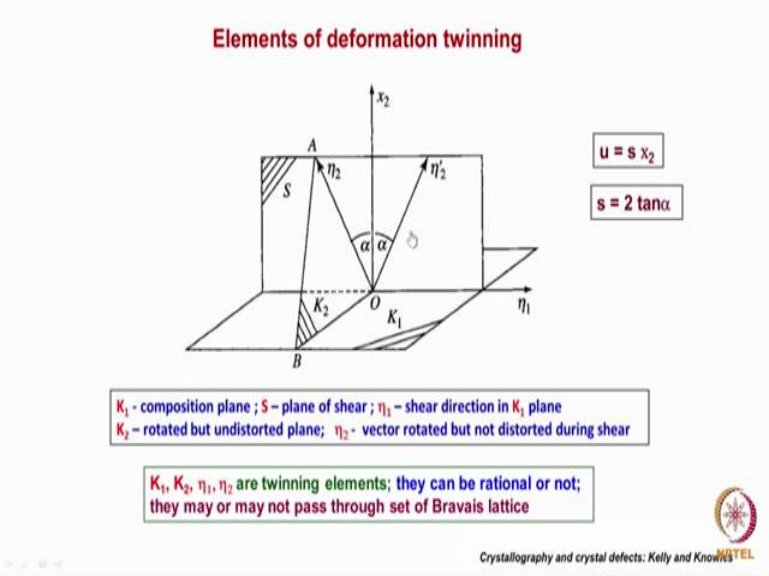

When we considered twins as a general phenomena of homogeneous deformation we understood that there are 2 planes are there, there is 1 plane which is called as a K 1 plane or a composition plane which is undistorted and unprotected. And there is another plane which is a undistorted, but it rotates during the shear homogenous shear transformation.

There same thing is being shown here in this slide where we are just showing K 1 plane and we assume that below this plane K 1 it is the material specimen which is not undergoing any shear transformation, above this its undergoing a shear transformation. The shear vector how we can calculate it if s is the shear vector which we can find out because if we know that vector which is rotated, but not deformed. What is the magnitude of this vector? Divided by 2 things, this height that will be giving their magnitude of the shear vector. If you know the shear vector then the displacement which is taking place at every point at any particular height from the composition plane we can calculate it using this formula. What is important to know is only these four quantities K 1, K 2, eta 1 and eta 2.

In addition to it, there is a plane which we call s, there is that plane is called as a plane of shear. So, the shear essentially this is the shear vector, there shear is taking place in this direction and the plane is normal to the K 1 plane these 2 vectors lying on a plane that is called as the shear plane. So, all the shear which we are measuring it is in this that is this

is a vector which is a initially in the unreformed material that during an homogeneous shear that transforms to it are 2 dash these called as a plane of shear s. So, the twinning elements are K 1, K 2, eta 1 and eta 2, that question is that has these planes have to be rational because normally whenever we conserve plane we conserve low index planes correct. It can so happen that sometimes plane may not pass through any particular plane.

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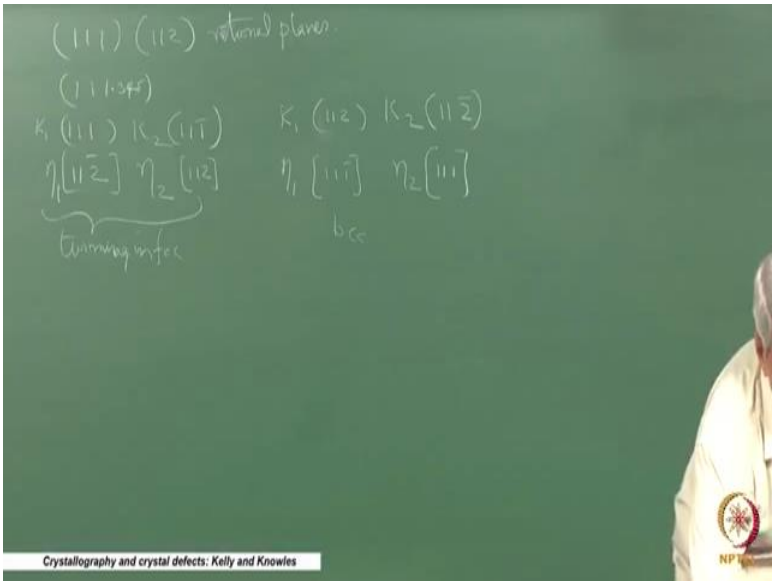

For example what can happen is that 1 1 1 or 1 1 2 these are all rational planes can. So, happen that is 1 1 1 point 3 4 5, if this is the sort of a vector which we get it these planes we call it as irrational planes; that means, that that plane may be a having a it will be a high index plane. Whenever we do microscopy when you work on stereogram then you get exactly that planes which quite often turns out to be non integer.

That in my well doing microscopy of not during microscopy after doing microscopy we will do an analysis of the fraction pattern and then we try to superimpose them on the image to find out the directions then we find that quite often something the planes will not be a rational plane.

Student: (Refer Time: 05:17) very some again specific means it may can be (Refer Time: 05:20).

It can happen in all materials.

Student: All materials.

All materials, these things are very common even in twinning there are many cases we are you can find it the plane shear rational. Now coming back to the subject. So, K 1, K 2, eta 1, eta 2 that can be rational or they can be irrational then another is that they may or may not pass through the Bravais lattice point that is if it is irrational many of them may not pass through the Bravais lattice point also. Let us consider the case where K 1 and eta 2 are rational. There are 4 vectors are there all of them could be rational, all of them could be rational or 2 of them as a pair we consider it K 1 and eta 2 rational.

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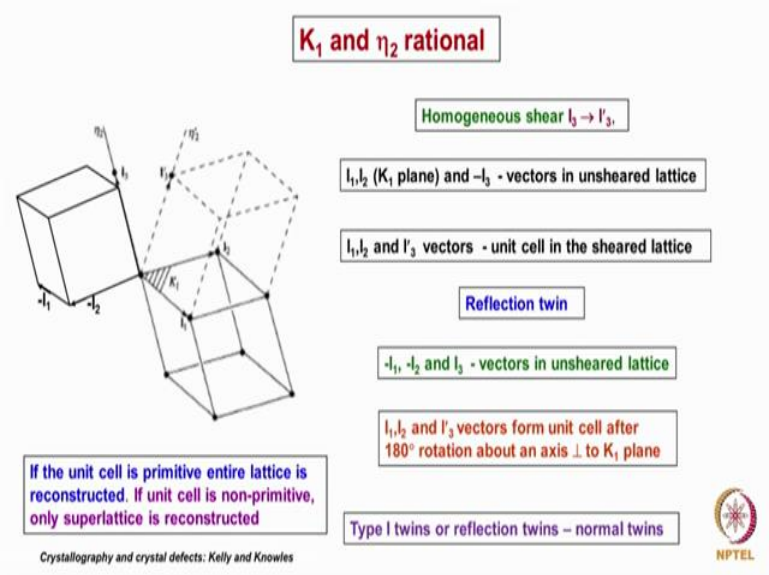

So; that means, that if K 1 is a rational plane index plane we can find 2 vectors in that plane which are lattice translation vectors, that let us consider them as l 1 and l 2. Eta 2 is also a rational direction; that means, that we can find a vector it represents a lattice translation vector that is what we have returned us l 3, if you take the negative of l 3, l 1, l 2 and l 3 this will represent the undeformed lattice correct or a unit cell of the undeformed lattice, and what does that shear do? That is when we apply a uniform shear in eta 1 direction essentially that moves from l 3 to l 3 dash that is what the atom is being shifted.

Now, if we consider l 1, l 2, l 3 dash is also now a vector it represents an atom point in the deformed lattice, these 3 vectors together define an another unit cell, these 2 unit cells if you look at it one on sitting on top of the other and it is nothing, but a it is a reflection twin, is it clear?

Student: But l 3 we I l 3 plane will equal.

Yeah equal. So, these 3 are, so these becomes a reflection twin. Other case which we consider it is that let us look at it, here what we have done it is that take a unit cell which is made up of minus l 1, minus l 2 and l 3 dash. This unit cell with respect to an axis which is perpendicular to K 1 plane if we dig given 180 degree rotation that will generate this unit cell that dash one; that means, that these are related by rotation.

So, there are 2 ways in which this twin could be generate that is one is a reflection and another is and 180 degree rotation about an axis perpendicular to K 1 plane these types of twins are called as type 1 twins, this is a normal (Refer Time: 09:01) which is used or they are called as reflection twins that is one or normal twins there are many ways in which because normal twins because there are related by 180 degree rotation around an axis normal to the K 1 plane. Reflection twins why they are calling it is because across the K 1 plane is a reflection is there. Here what we have done this we have assumed that K 1 and eta 2 are rational.

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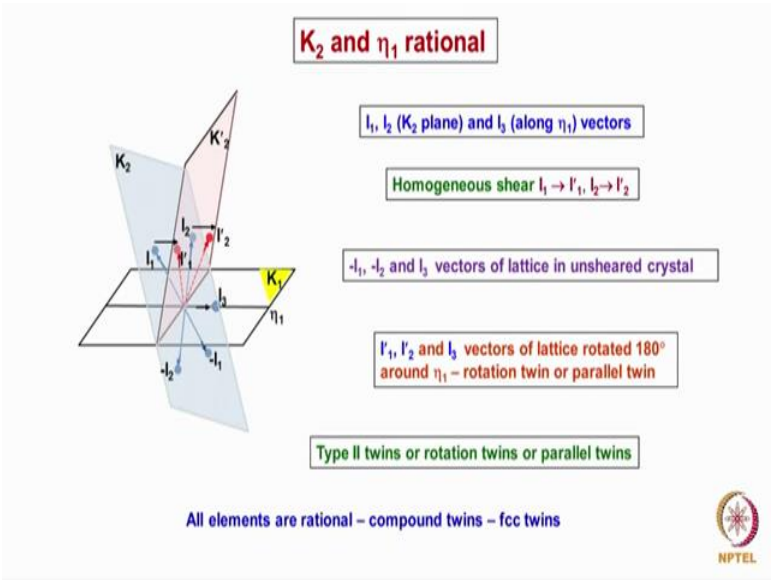

Now, let us consider the case K 2 and eta 1 are rational here what I had shown is the projection of the various planes, this is K 1 plane, eta 1 is the shear direction in the K 1 plane, assume that the; and l 1 and l 2 are 2 vectors like the way we considered earlier when K 2 is a rational thing we can find some 2 unit vectors in the K 1 and K 2 plane smaller, not even to small vector lattice translation vectors. These 2 vectors may

represent a primitive lattice are they need not and another thing also which we have to consider it is the that a its easy to find only when that K 2 plane is a rational plane or K 1 plane is a rational plane these vectors are you get other way the victors will be at a very long will have a very large magnitude. We have 2 vectors l 1 and l 2.

If we take these 2 vectors by a shear what essentially happens l 1 transforms to l 1 dash l 2 by the application of the shear transforms to l 2 dash, correct. In the shear lattice this will be the position of the vectors right l 1 and l 2 if we consider it that minus of l 1 and minus of l 2 and l 3 is a since eta 1 is a rational direction there can be a lattice translation vector in that direction which is l 3; minus l 1 minus l 2 and l 3 now represent a unit cell correct, the unsheared lattice.

Now, if we consider to this unit cell if we give a rotation by 180 degree around eta 1 direction then l 1 will become l 1 dash, minus l 1 become l 1 dash, minus l 2 become l 2 dash l 3 dash remain by 180. So, essentially this is another type of a twin which is occurring. This we need generator though we are applying shear crystallography when we consider it this is like the bottom half around the composition plane in the direction of the shear if you give a 180 degree rotation you can generate the other part of the crystal. These twins are called as rotation twins or parallel twins or that other is this called us type 2 twins because the parallel twins a all these notations are used by neurologist. Crystallography this called type 1, type 2 there are some further subdivisions are there which we will not go into.

Suppose all the elements K 1, K 2, K 3; K 1, K 2, eta 1, eta 2 all of them are rational then this is called as a compound twin. Compound twin essentially means that whichever way you consider it either by a reflection or by a rotation around an axis normal to K 1 plane or rotation around an axis rotation around the shear direction if you take it all of them generate the same type of a twin.

Student: (Refer Time: 13:36).

No, for example, in FCC if we consider 1 1 1 K 1, K 2 can be 1 1 1 bar, eta 1 can be 1 1 2 bar, each are 2 can be 1 1 2. So, these are all rational once this generates a compound twin. Similar type of compound twin is generated in the case of BCC also. We will just come to that.

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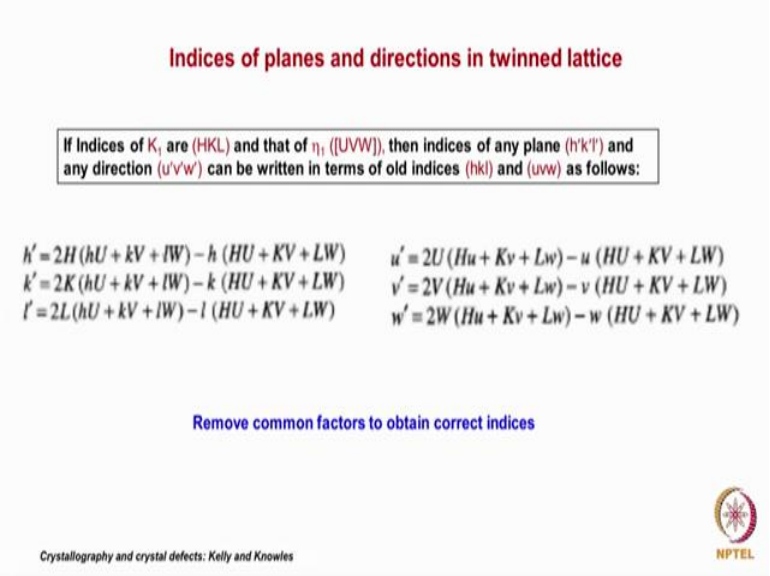

Before that let us look at indices of the planes and directions in the transform lattice we have studied earlier the lattice correspondent and using that when we crystal undergoes a transformation from one structure to another structure or from one orientation to another orientation how to find out the directions also indices of the plane. Exactly using that same methodology we can find out indices of the planes and the direction in the deformed lattice in terms of the original unsheared lattice. So, here what we are considered K 1 suppose it has got HKL capital HKL we have written that is that indices of the K 1 plane then that of the direction is UVW K hat 3 1 and if you know that indices of any direction that is h dash, k dash, l dash is in the sheared lattice in terms of HKL can be found out using these formulas which are given.

When we use these formulas and try to find out sometimes we find that there will be some common factors which we have to remove and that way we can get information about which direction in the deformed lattice corresponds to which direction in the undeformed lattice.

Now let us consider twinning in BCC twinning in BCC we considered when we discussed about dislocations in BCC is a structure. The same thing which we are trying to show here and that BCC twins are observed on 112 plane, and 111 is the shear direction that is what essentially is being shown here.

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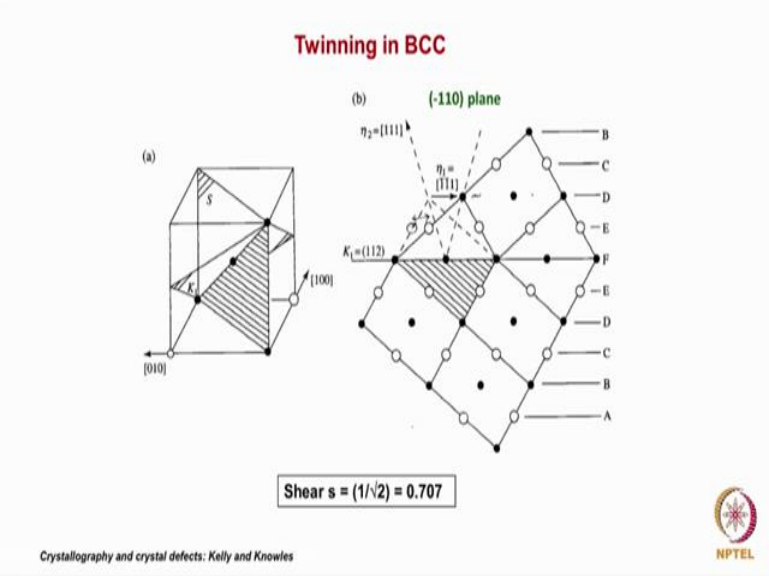

And the stacking sequence in a 112 direction is essentially a six layer stacking sequence A B C D E F. Here by a moment of here by fix 1 on 1 partial and every plane it can change the stacking sequence from A B C D E F to E F D C B A that way a twin could be generated. What is the twinning shear which is required in this case that one can calculate which I had mentioned earlier? That if you know the length of the vector which has rotated from undeformed lattice to the deform lattice that is only which is underground rotation, if you know the displacement which has taken place from one end to the other end and divided by the height from the K 1 plane if you take it then we can find out the shear vector.

In the case of twinning in BCC the shear turns out to be around 0.707 it is a very large here. Exactly the same shear which we have seen that it is required in the case of FCC also. So, essentially what happens here K 1 equals 112, K 2 equals, eta 2 equals if you look at the indices they are just reverse between the planes and direction between which is for a twinning in FCC, these are twinning elements in BCC lattice. So far we have considered the symbol lattices; let us look other types of crystal which are not cubic or even in cubic which are ordered ones.

Let us take the case of a thing Zinc Sphalerite. Zinc Sphalerite essentially has Bravais lattices face centered cubic and its space group is 4 bar 3 m.

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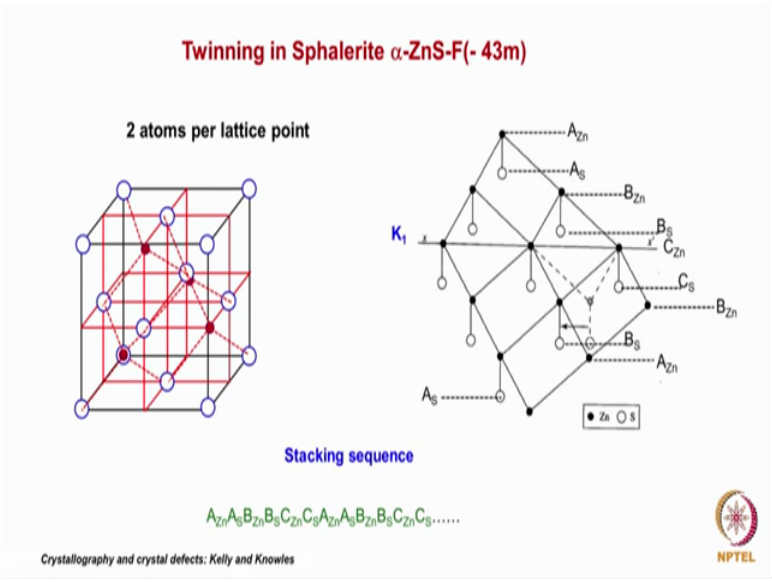

The crystal structure of Zinc Sphalerite is shown. Here if you look at the stacking sequence along 111 plane it is as its being mentioned A F sink 11 on 1 layer just above that another a layer of sulfur then the B layer of sink, B layer of sulfur this is the way to will go. So, that the stoichimetry as to be maintained. The same stacking arrangement is shown in it 111 bar 0 production plane, like what has been since it is FCC and that same plane we can show. Here if you look at it this is a sink plane, then comes a sulfur plane, then B sink plane, B sulfur plane like that its going here what is being shown is we are showing a projection of part of this undeformed lattice into the reform region.

And the shear is from here to here in this direction. So, the shear what it does it is that it moves all the atoms from here to here, the next layer B layer and that this is also being B layer of sulfur is also being moved from here to here like that they are moved that way this is the sort of a structured which it form. If you look at this structure that is the homogeneous here has occurred along the eta 1 direction and that is what has lead to this deformed structure is none another orientation. If you look at these structure immediately one can notice it that across the composition plane there is no reflection correct, it does not get reflected.

But at the same thing if you look, took a plane, took a direction which is perpendicular to the K 1 plane if you take a 180 degree rotation around that plane that integer is generated. So, essentially that which is there is a subtle difference between the various

twins when we consider different types of ordered lattices then we can make out why all these operations which we discussed earlier each of them are important, each produces a different type of a twin.

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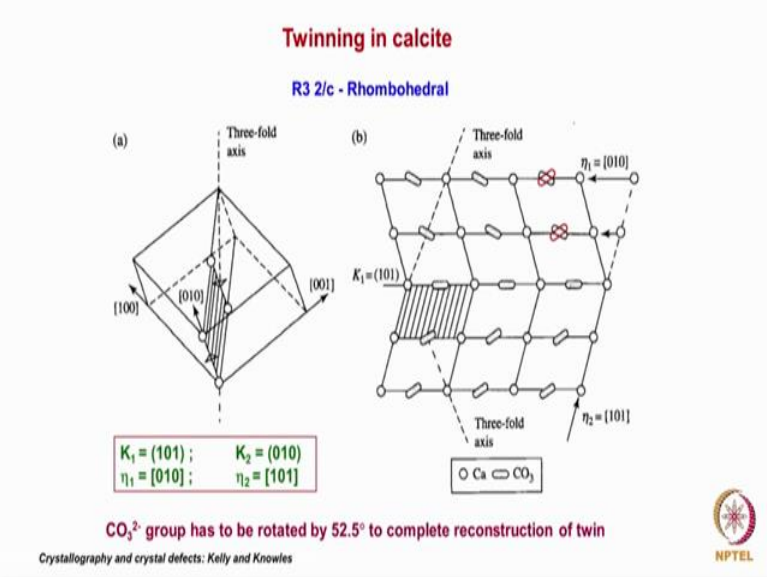

So, this is just nothing, but a rotation twin. Another case which we are considering it is twinning in calcite, calcite is calcium carbonate. It has a rhombohedral structure. The unit cell of calcite it is being shown and the twinning elements are K 1 is 101 and K 2 is 010, then eta 1 is a 010 and eta 2 is 101 bar these are all rational indices. Here what is interesting is that the CO 3 that group is inclined in this way in the unit cell that is what essentially is being shown here in this particular fashion.

Now, when we homogeneous shear is being applied as you can make out this essentially will be tilter and it will be in the one the red one shows in that weight has to be. If remains in that way if we across the K 1 plane if we consider the reflection is it is not a mirror image of that bottom half. So, if it has to become a mirror image of the bottom half this part of it has to be rotated only the CO 3 group has to be rotated by around 52.5 degrees that is from the crystallography which we consider, if such a rotation is not given that wind region cannot be observed, but twinning is being observed in the material it is a reflection to in it appears right. So, what we are trying to do is that from a crystallographic consideration how can we explain this; that means, that the homogeneous shear essentially deforms the Bravais lattice, but still some of the

molecules require some reorientation to generate a twin. These process will be occurring simultaneously in the material. So, what we are trying to do is how to explain this correct, this is the way a crystallographic will we try to explain.

Let us consider because another important material like BCC and FCC structures SEP structure is also an important crystal structure where many elements crystallize into SEP structure and they are all structurally very important material. Here as I mentioned earlier in that when I talked about zirconium that only four independence slip systems are there; that means, that to maintain the continuity.

Student: One.

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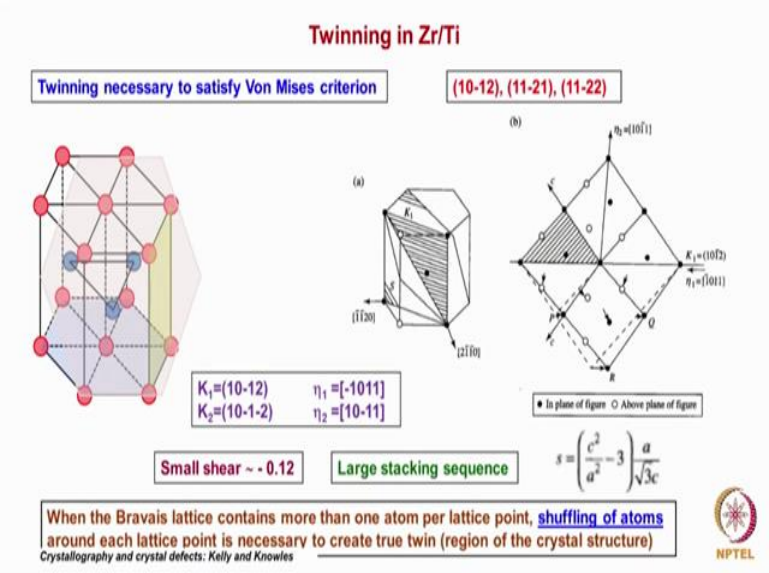

(Refer Time: 25:06) mentioned we request 5. So, twinning is one of the slip system which can (Refer Time: 25:11). The common slip systems which are been seen in siliconeum and titanium are 1101 bar 2, 112 bar 1, 112 bar 2 these are all the planes over which twinning has been observed. But it is going in this is the one which is most frequently used 101 bar 2 the others are less frequently seen and these are all the twinning elements K 1, K 2, eta 1 and eta 2. Like this way we considered for all of the crystals. Here also if you look at this structure the projection along I am a plane that is projection of the shear plane is being shown the projection of the entire unit cell deformed and undeformed on the shear plane we are showing it.

Here if you look at it this is very interesting because in this structure hexagonal close packed is not a Bravais lattice. If something is not a Bravais lattice all that twinning which we are talking about this with respect to a Bravais lattice. We can have atoms around each of the lattice point cross structure which are put together, but to maintain that identical position they will not be getting deformed in most of the cases they will be remaining as such like these. So, that is what essentially happens let us see this case this is essentially the projection of the undeformed lattice it is shown here and if you see from this position it is being shifted here, this position it is being shifted here, this position it is being shifted here, this is essentially for the Bravais lattice which is happening because hexagonal close packed structure can be considered as a simple hexagon with 2 attempts per lattice point.

Then what happens is that many of the positions of the atoms like these ones or these ones they come to positions which are wrong position. What has been seen is that the twinning and such when it has been observed it shows a true twin; that means, that to get a reflection twin, these positions have to shuffle across a little bit to reach the correct position. So, in twinning shuffle is one of the important component which has to occur along with the sharing of the Bravais lattice and in this particular case the shear is extremely smart of the order of about point 1 2 whereas, one should remember that in the case of FCC and BCC its around 0.707 and when the shear is very small it is that one can calculate what is the stacking sequence here is a large stacking sequence and using this formula, this formula from crystal structure one can derive it I am just giving only the formula, using this one can find out what the shear vector is. The shear vector depending upon these values it could be positive or negative also it can turn out to be.

So, essentially what is important if that when Bravais lattice contains more than 1 atom per lattice point most of the cases shuffle is also required. So far we are contains few special cases, but all these cases just to prove some view point – one, that only in the case of lattices our primitive lattices are where the Bravais, or Bravais lattice. In those wont to twinning occurs it is essentially a type of a compound type of twin which you have noticed in FCC and BCC where shuffle not rotation is necessary.

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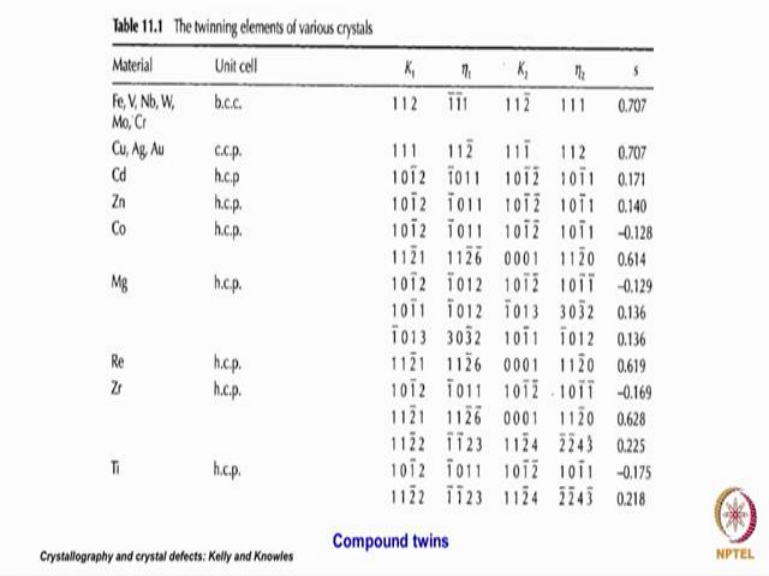

In other lattices we require rotation as well as the shuffle is required here what I am showing it is essentially twinning elements in the various crystal system.

Some examples are like in iron which are all BCC iron, vanadium, niobium, tungsten these are all BCC system model the twinning elements and what all that, shear also which is required to generate these twins. Similar in h c p copper, gold; no, that is FCC copper, silver, gold and similarly all the h c p structures. We can see that especially in a h c p structures some of them like in the case of rhenium it requires a 0.619 shear whereas, in the case of many other elements like titanium or zirconium or in magnesium or in cobalt a small shear is required and this shear vector also which should remember that what we have considered here there shear is along the specific K 1 K 2 (Refer Time: 31:05). This is not the only plane in which here can occur because as we can see there are many planes are like in zirconium there are many K 1 and K 2 planes are there.

If you look at each of these planes the quantum of here which is required is going to be different, this I had already mentioned.

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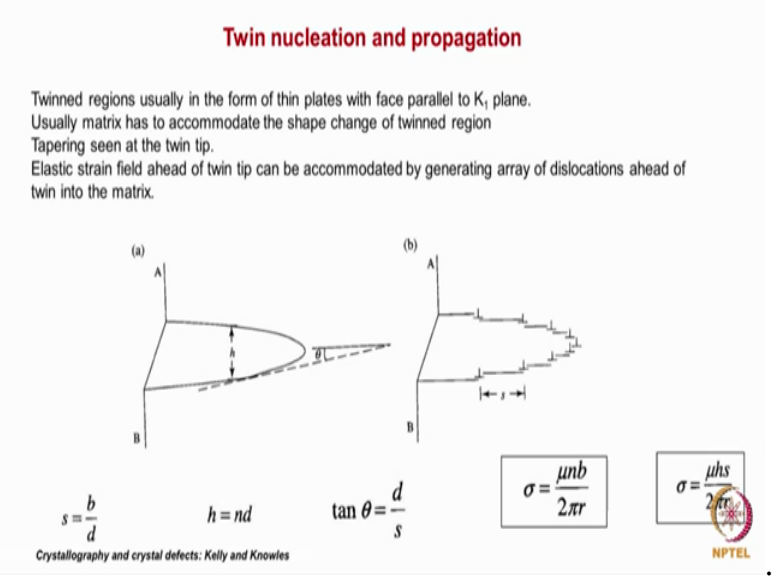

So, so far what we had considered as twinning in a Bravais lattice how we can understand it using crystallography and homogeneous deformation. When this sort of a sharing process leads to orientation of another orientation of the crystal they are essentially, they related by either reflection rotation or inversion. Quite often these shear transformations can be considered as not only just shear, but also shuffle or rotation of some positions are required. So, (Refer Time: 32:11) crystallography is concerned, we have never looked at how the nucleus of the twin form how it propagates correct. Let us look at the twin nucleation itself.

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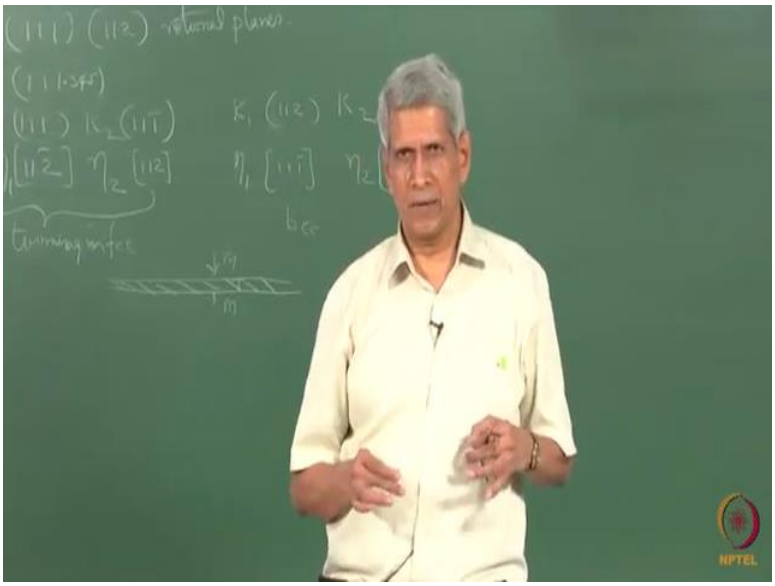

Generally since the shear is very high which is for twinning, generally when the twins form they form is very thin plate and propagate, this interface between the twin region this is twin this is the matrix this is the either the composition plane of the twinning plane and generally this is called as a coherent plane, it is a highly coherent plane and the energy the twin boundary energy is extremely smart for this plane. But as the twin has to propagate into the material they heard of the twin that is a large it is a shear is very high shear which it has to accommodate; that means, that this shear can generate classic deformation or the same classic deform accommodated by, this shear can be accommodated by generating dislocation ahead of the twin tip and not only that generally in such cases this tip will always turned out to be essentially a tapered one. So that is what essentially is being shown.

In this specific case if you consider it we have a, if you look at the surface of this one when we apply a stress from here this much region has essentially started to forming and it is like a tapered one that propagate. Well, if we know the height of this twin layer which has formed and from that height to the tip what is the distance we can calculate, how many dislocations which have to be generated to accommodate this string corresponding to the twin that is what essentially has been done and also that when these dislocations are generated what will be the stress which will be corresponding to that much number of dislocations are generated and if we move, what is the stress I heard of

that on the first dislocation that is what we are trying to calculate here. This is exactly what is being shown.

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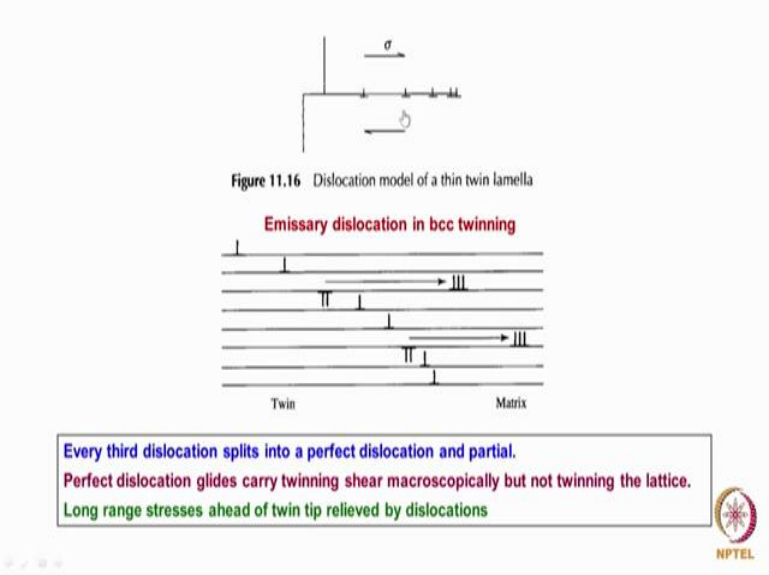

Here, if you see that the region which is getting shared a lot of dislocations which are being generated, this can essentially happen or it can happen that instead twins could be generated over the entire region that is like what is being shown here, here, here, here, dislocations are generated at this is like a small step which forms. So, that all these planes could be region in between could be coherent in boundary. So, that the energy of the boundary is reduced.

In bcc what has been seen is that the perfect dislocations of the type a by 2111 is punch out and then when they are punching out this reaction which we have considered earlier, when one dislocation is being punched out that another dislocation with a sign which is negative of that if it is there that can be a by 6112, a by 6112 type.

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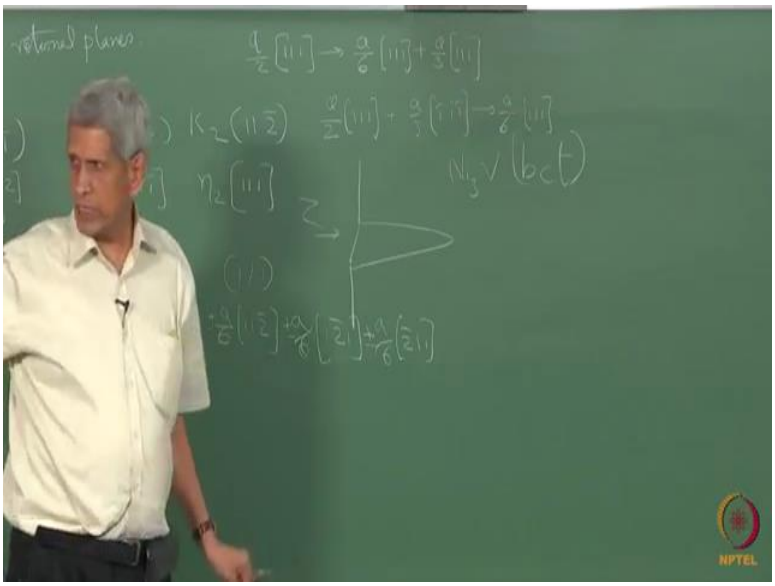

So, essentially we can write you can write the reaction of this time; that means, that if a dislocation of this type or this type is getting stuck at that material this reaction if you write it the other way around, the shear which is corresponding to it is say by 6111 then this can be correct, this gives a by 6 this is the shear which is required on every layer to generate a twin in bcc.

So, what we are doing it is that a perfect dislocation plus and another dislocation of this type this dislocation can get stuck at the interface and this dislocation can be generated. In fact, it has been seen that because in BCC dislocations of these type partials are not generated that has not been observed we can only perfect dislocations are seen, but it can be those dislocations can be generated as a result of this sort of a reaction where some dislocations are getting stuck at the interface. That is what I had mentioned that a way third dislocation splits into a perfect dislocation and partial. Now perfect this location glides carrying the shear microscopically, but not the twinning lattice, but because of this long range stresses which are introduced are relieved by the moment of these dislocations.

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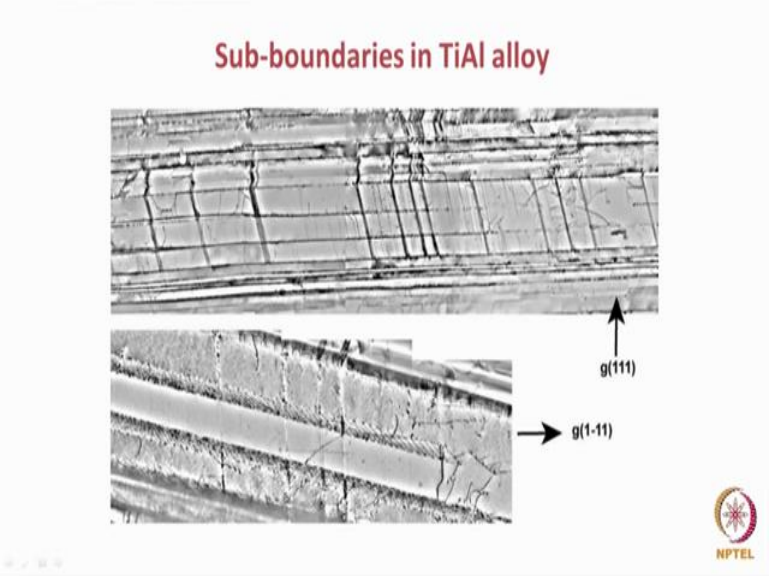

Here what I am showing it is essentially in a titanium aluminum alloy. If you look carefully in this region is a twin which is within 1 gamma lamellae, one can notice it that the twin tapers down, yes tapering could be observed here then head of it if you look at it lot of dislocations are this location arrays and I think this is a twin which is receding here in this case, but one can say that that lot of dislocations are there heard of it which is punched tone this is certain inclined one, orientation of the twin, one can see that this location arrays could be observed very clearly.

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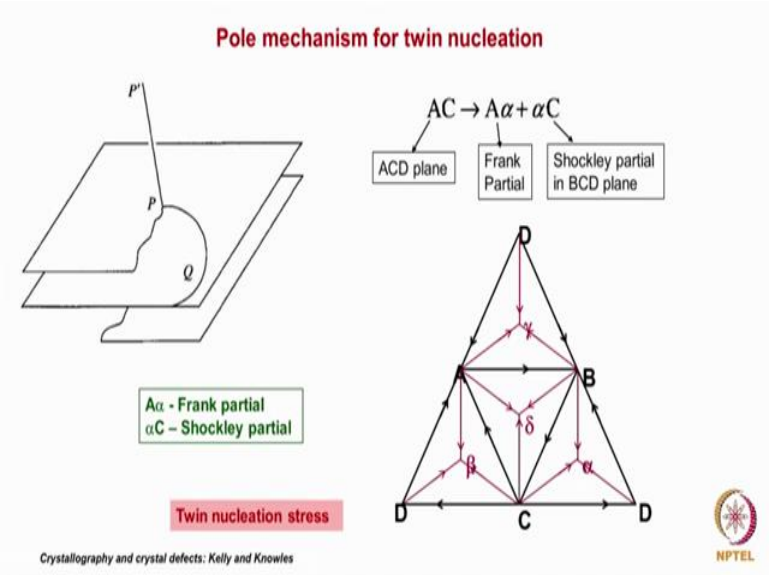

So this is one way in which a twin could be nucleated that enters region is getting deformed. The another one which happens is that what is the mechanism by which like in the case of FCC, what is the way in which we know that the sagging fault energy is small one is overlapping sagging fault can be raised to twin, is there any other mechanism by which a twinning could be generated from a single dislocation. One of the mechanism which has been put forward is called as the whole mechanism for twinning. Here what is essentially considered is that yeah this location like AC it is a perfect this location that splitting into as a component A alpha which is a frank dislocation plus alpha C which is essentially a Shockley partial in this plane.

The advantage with this a sort of a dislocation reaction is that the A alpha the burgers vector is a out of the slip plane, alpha C is in the slip plane because of it if that dislocation slips on this plane. Like the configuration which is being shown P P dash every rotation which it takes in the perpendicular direction the burgers vector if there it will be shifted by 1 layer, so it will be generating streaking fault on every layer that is how it will, that way we can consider that twin is generated in FCC material correct.

That is here otherwise every layer twin has to be generated that is every layer a partial has to be generated whose propagation generates overlapping a faults which gives rise to twin that is one mechanism. Is that what we are looking at it, either another mechanism by which a single dislocation which is there that itself can generate fault on every layer this is one mechanism by which it could occur.

Then in addition twin there are other types of twins which are there which are called as elastic twins that has been seen in many materials, especially even in I think calcite it is being seen. What happens is that due apply a stress like in this case it twin is generated, stress is being applied to accommodate the stress twin is generated, you remove the stress the twin will vanish it will come back to original position. Then another is what is called as an anti twinning these are all some terminologies which are used, anti twinning essentially means that in BCC stress if we consider, in a one particular direction that vector a by 6111 moves, it generates a twin.

Let us look at that direction opposite it a by 6 1 bar 1 bar 1 bar that does not generate a twin it is (Refer Time: 42:46) high energy this one and generally what happens is that in such cases generally they give rise to dislocation motion and not twin and this requires

very high stress also. These are called us anti twinning. Then micro twins, micro twins as I mentioned yeah micro twins has from the word itself we can understand they are very small twins, generally during growth of a copper or gold from vapour phase when they grow many of these fine nano particles they are formed, one can always observe a lot of twins within them these are called as micro twinning.

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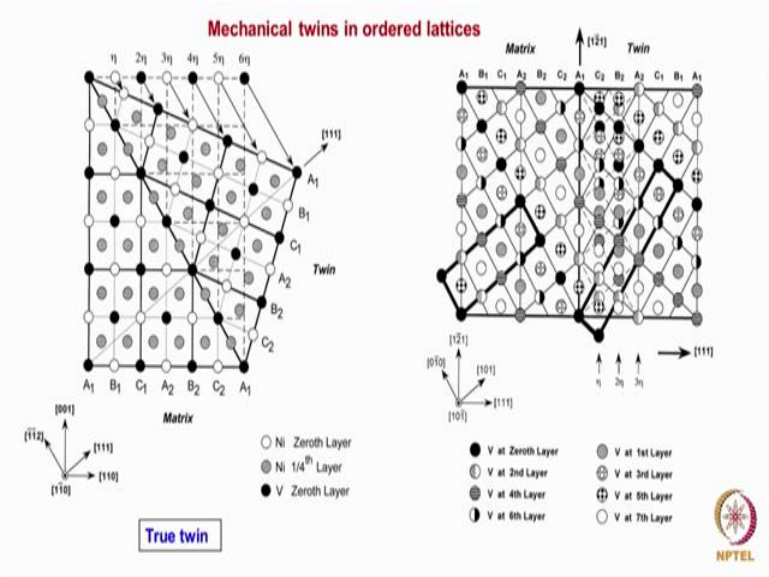

Then there is another terminology which is used as pseudo twinning. The pseudo twinning is one which is seen in many ordered alloys. I will just show one example this is a twinning in a structure which is called as a gamma double plane, these phase forms in many nickel based super alloys other than that nickel 3 vanadium has this structure Ni 3 V. Crystal structure is body centered tetragonal. This I had shown this structure earlier and in this 111 plane is the one in which a twinning occurs. The stacking sequences essentially A B C, A B C it is not a 3 layer, it is a 6 layer stacking sequence what is essentially important is that here by moment of a partial a by 6 111, a by 6 112 on every plane we can generate a twin and if you look at this, this twins are essentially true twins; true twins means that the ordered lattice is being retained.

But in some other plane, in some other vector because here we have considered one particular vector in another direction because if we consider 111 plane we can have a partial 2 bar 11 these are all the partials which are possible. In fact, only 1 particular partial only generates this 2 twin the other partials if they are passing through they

generate a different type of a crystal structure, but if you look at the atom positions with respect or disordered lattice the twinning has happened, but in the ordered lattice since atoms occupied different positions that becomes very clear if you look here because we have constructed a unit cell in the undeformed lattice and when we try to construct a unit cell in the deformed lattice it has a different unit cell different type; that means, that it goes into a different transformation is occurring these type of twinning is called as pseudo twinning.

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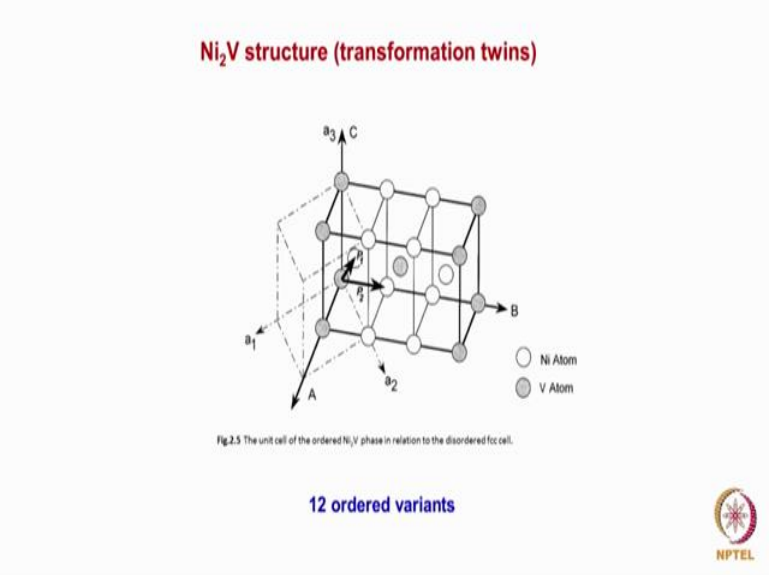

This is another structure, but we will not go into all these structures, I can show examples where a twinning occurs in ordered a structure. Especially in ordered structures we can have 2 terminologies which we use one is called as 2 twin where the ordering of the disorder the ordering of the lattice is being retained after twinning in the twin lattice also, another is called a pseudo twinning where the ordering is not being maintained.

So, essentially what we have discussed so far is weight twinning is necessary because in many materials, because twinning is an alternate mode of deformation and when slip is not possible twin is one mode by which information can take this. The second one which we looked at it is that given during growth of crystals twin nuclei can form because of the probability, because there are different orientations are possible. So, these orientations can be related by a different symmetry relationship of either rotation reflection of inversion they are called that either growth twins and they are called as

transformation twins or orientation twins and then mechanical twinning that is what we deform a material when deformation is inhibited twinning can form in many materials that also we have looked at it.

And then also we have seen that when twinning is occurring in some cases when it is a Bravais lattice which is a, that is the number of lattice points per unit cell is 1 and then it is the all the lattice point are shear then other cases where the number of lattice point, the number of atoms per lattice point is more than 1 in such cases some shuffles or every orientations are necessary that is when we consider the crystallography of twinning as of homogeneous shear.

So, we will stop it here. Essentially all the basic features about twinning, has been covered in these 2 classes.