Materials Science and Engineering
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Lecture – 11
Crystallographic Defects

Hello, friends. After going through microstructure metallography microscope let us go in a slightly different direction and now, we will want to see or we want to discuss that what kind of defects are there in the crystal ok. So, crystal we have already seen ok, now, we want to understand that there may be some defects in the these crystals and what type of defects these are. So, this is just a animation to I am trying to create a defect here in the word itself.

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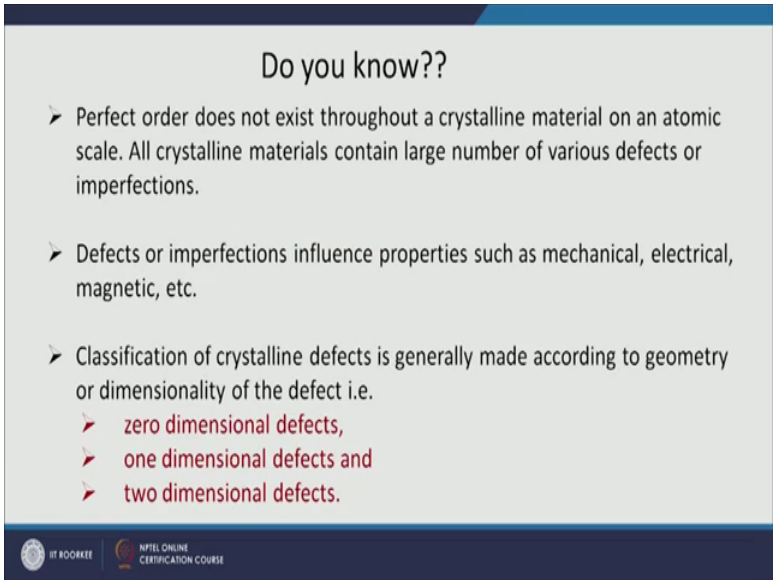

So, basically till now when we were discussing the crystal structures and the lattice, we placed atom at each lattice point; Thinking that all the lattice points will be occupied by atoms or may be compound and so on ok. But, in general any real crystal if you see it will contain large number of defects ok, it will have and of course, these defects also affect the mechanical, electrical, magnetic properties. In fact, most of the metallurgy or study of materials engineering is basically how to understand these defects, how to manipulate this defects and how to use these defects for our benefit. In fact, a material

without defects is a very boring material ok. I do not like a material which does not a does not have any defect.

So, any material in, in fact, its use is based on what kind of defects are there in and I can manipulate I can tailor the properties of the material by manipulating the defects ok. So, defects are very important they are not bad ok. The defects are very important for understanding of materials and as well as how I can design new materials by taking help of these defects.

If I want to quantify the defects the defects are basically quantified on based on their geometry and they are either called zero dimensional defects, one dimensional defects or two dimensional defects and 3 volume defects also, but we are not talking about those defects in this particular lecture, because we are interested in the defects which are related to crystals or which are guided by the crystals.

So, these are the three broad types of defects which are going to be there and we want to study these defects.

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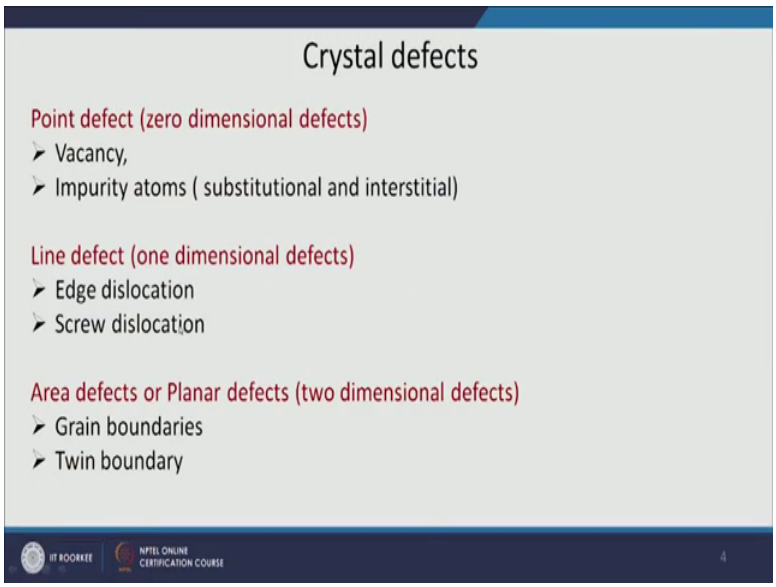

Again, in each of these category we can have different type of defects for example, point defects which is basically a zero dimensional defect it does not have it is the point no dimension ok. So, in that you will have a vacancy or you can have impurity atoms

impurity or sometime you can call them this alloy alloying elements these are the either substitutional or interstitial we will see what do what do we mean by these two terms.

Then there can be a line defect which is a one dimensional defect ok. In that you will have edge dislocation or the screw dislocation again we will see what do we mean by these terms and what do we mean by dislocation itself. Then, there will be area defects or planar defects 2 dimensional in nature and grain boundaries we already now know this term grain boundary we have discussed that quite for some time and another is twin boundary ok. So, again we will see what do we mean by a twin boundary.

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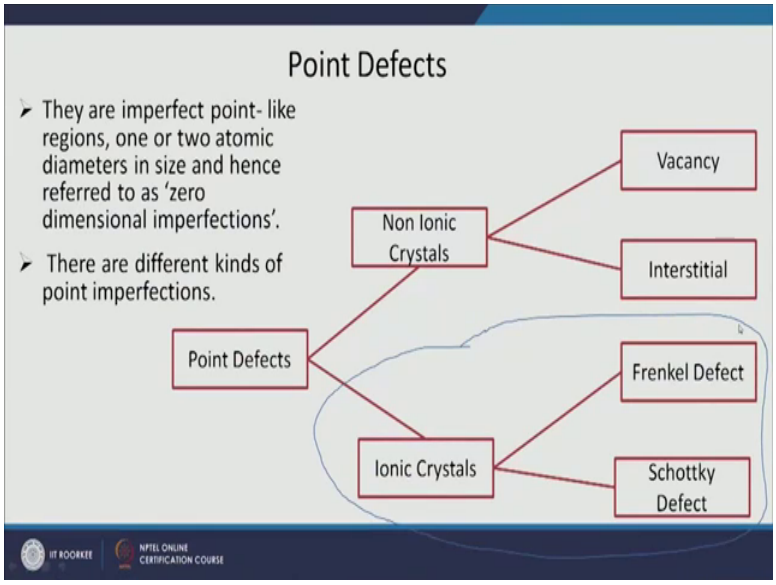

Now, coming to point defects you can classify them in these two types actually this in circled one I am not covering right now, because these are mostly you will find in ceramics and they are of not interest to a mechanical engineer as I understand. So, we will be mostly concentrating in a the defects which you will find in a nonionic crystal ok.

So, basically point defects if you want to see they are imperfect point like region basically 1 or 2 atomic diameter in size and that is why they are referred as zero dimensional imperfection and there are different kind of point for imperfections, so, there is nonionic ionic. In ionic you have Frenkel defects and Schottky which we are not going to cover here, but if you are interested in any material science book you will be able to see these defects ok, but we will be mostly interested in these 2 defect which are of zero dimensional in nature.

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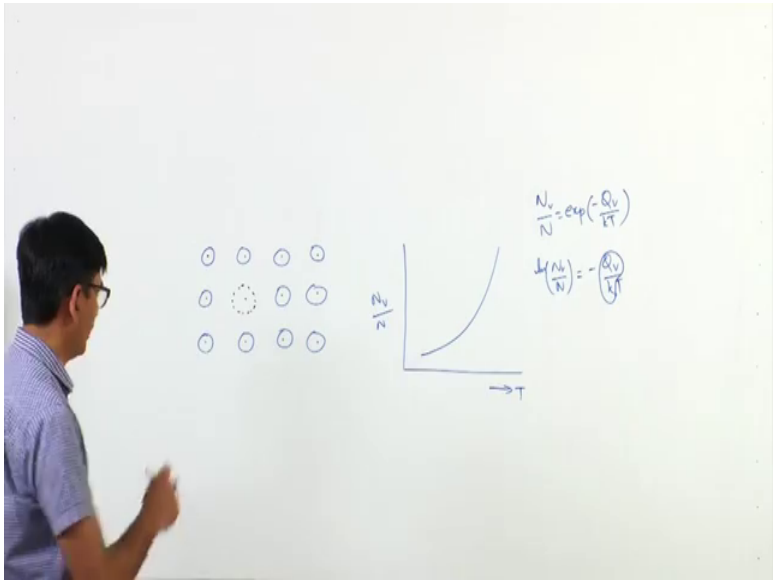

So, if you want to see vacancy means in the regular arrangement. So, you have lattice points and on each lattice point you should have an atom. So, suppose this is a lattice and of course, as we have already discussed in or crystal when we were discussing crystals that you on each lattice point I am putting an atom here.

So, vacancies when one of these atoms is missing from the lattice point. So, for example, this atom is not there ok. So, the lattice point is there of course,, but the atom is missing from that. So, they there is a vacancy now. There is no atom there. So, this is called a vacancy. How they are create created? they are created by thermal excitation.

So, when the temperature increases what happens all these atom vibrate on their mean position. And, in this process sometime atom will get enough energy to break all the bonds from the surrounding atoms. So, this atom for example, was having bonds with this one this one this one and this one ok. So, it broke all the bond and came out of this lattice point and started roaming around and left a vacancy behind.

So, this is actually a temperature dependent phenomenon.

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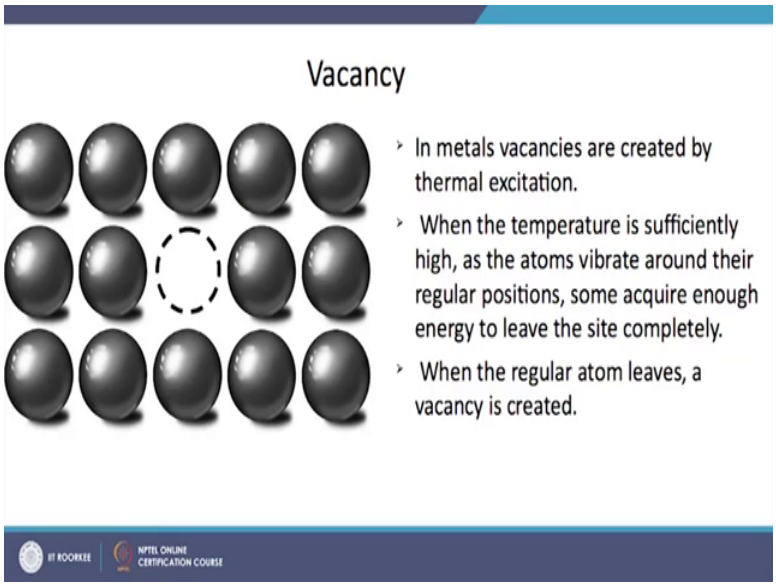

So, when the temperature is sufficient and they vibrate they gets some time they get acquire sufficient energy to break free and when they do that it is called vacancy. Now, most important you can say quality of this defect which is called vacancy is that this is a thermodynamic defect. This is the only defect which is a thermodynamic defect.

The meaning of thermodynamic defect is that it is you can find it that what will be the quantity of this defect in a particular material only by knowing the temperature and it is dictated only by the temperature. So, I cannot increase or decrease the number of vacancies in the material ok. It will be dictated only by the at what temperature my material is at that particular point. So, it is a function of temperature only ok.

If you see other defects these defects you can increase or decrease by doing certain for example, some deformation or maybe by doing some kind of heat treatment whereas, in vacancy it is only dependent on temperature and I cannot increase or decrease according to my will ok. So, this is the only thermodynamic defect which is very important ok.

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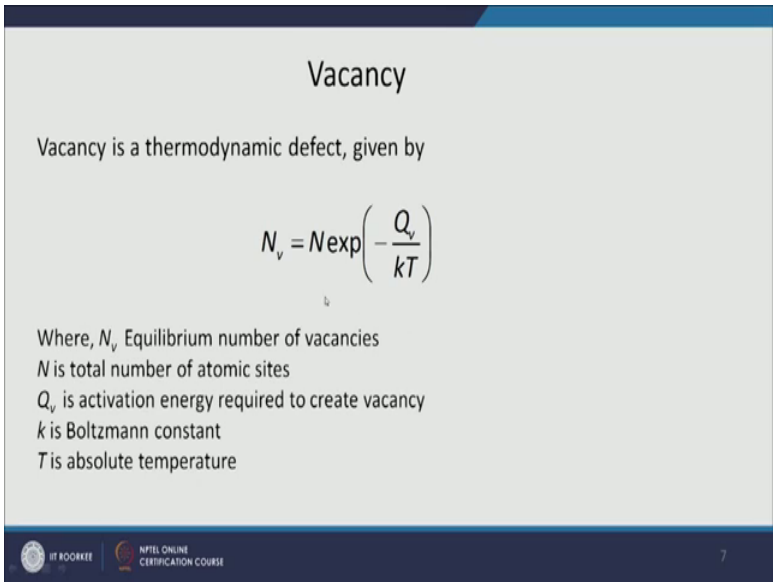

And, the number of vacancies will be given by a relationship erroneous of relationship where N v is the number of vacancies ok. So, in this case it is 1 N will be the number of lattice points on which you should have atoms or atomic sites which in this case you can see that there are 12 sites like that and exponential minus Q v is your activation energy which is required to create the vacancy. So, basically it is related to the bonds how much energy will be required to break all the bonds and take out the atom, k is Boltzmann constant and T is your absolute temperature.

So, if I want to know that what is the number of vacancy will be there at a given temperature basically, if you this is the exponential relationship if I plot this relationship ok. So, function of temperature it will increase something like this.

Another interesting thing is that if I rearrange this equation then it this equation will be like this and because this is the exponential equation if I take logarithmic on both the side it will be. So, it looks like a equation of a straight line where this is why this particular term is m and 1 by T is x.

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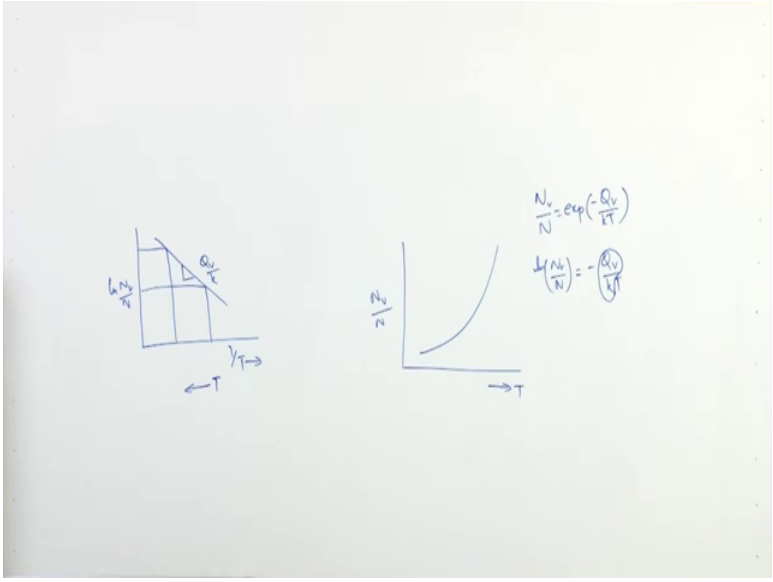

So, if I plot now this 1 by T as a function of logarithmic of N v by N. So, this is log of N v by N. And, this is 1 by T ok, then you will get a line of negative slope because there is a negative term there and the slope of this line will be equal to Q v by k. So, by knowing that how the number vacancies number of vacancies are changing as a function of 1 by T and by the slope I can get what will be the activation energy.

Or, if I know the activation energy I can tell you at a at a particular temperature what will be the number of vacancies will be there. So, 1 by T if it is increasing here, that means, T is increasing in this direction. So, at a higher temperature, I will have more vacancies, at lower temperature I will have less vacancies, at 0 Kelvin I will have no vacancies. So, at only 0 Kelvin you will have a material without any vacancies at any other temperature the material will have some vacancies in the and these are called equilibrium concentration of vacancies ok.

Then another type of point defect is called interstitial defect in which case an atom will come and occupy a interstitial position.

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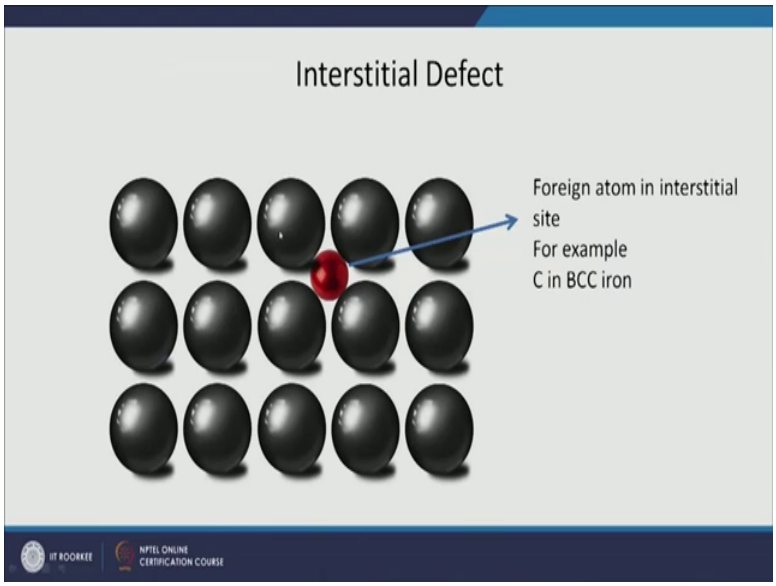

Interstitial means in between these two, four lattice points there are atoms on those 4 lattice points there is still some gap is available for every small atom to go and sit there. So, this site is called interstitial sites a small atom can go and sit there ok.

For example in BCC iron carbon is a interstitial an atom which is a very small atom it goes and sit in the interstitial position of course, this is a different arrangement than BCC. In BCC you will have different interstitial sites and the carbon will go and sit in those interstitial sites. So, this is called an interstitial defect. So, vacancy is basically you just take out an atom from it is site, interstitial means a foreign atom will come and sit in the interstitial position.

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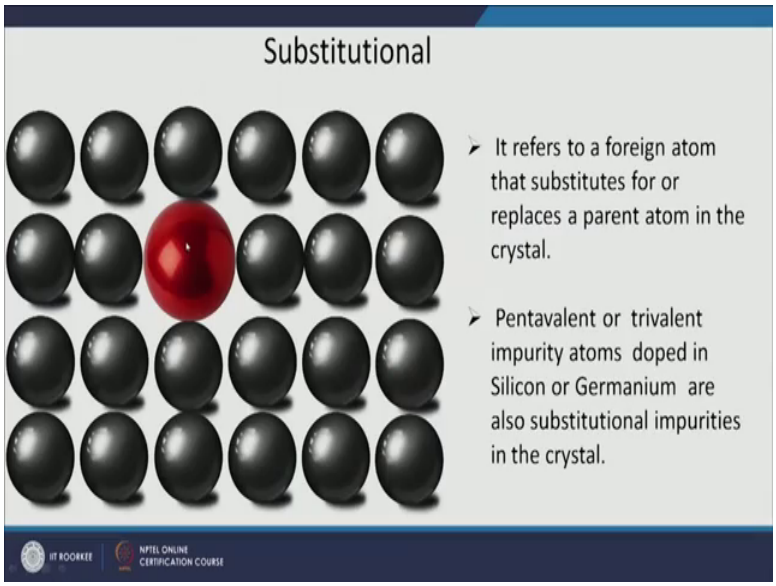

Now, instead of vacancy you can also have a condition where a foreign atom comes and occupies the normal lattice site. So, earlier we saw that I can have vacancies.

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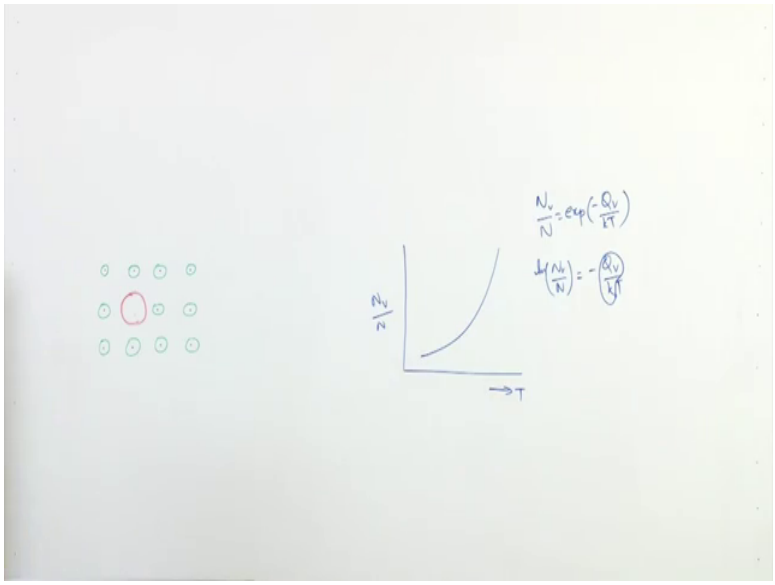

So, suppose these are the lattice points and atoms are there on each of these lattice points. So, one case was that I said you can have a condition where this atom is missing from this side it is called vacancy. There can be another condition where another atom comes and sit in on this side and of course, the site of the size of another m atom which

is foreign atom which is coming can be small than the earlier one or it can be a bigger one something like this it is coming and sitting.

So, it is substituting the parent atom which is already there a host atom and it is going and sitting there, that is why it is called substitutional defect or substitutional impurity atom, because it is replacing the host atom and sitting. Whereas, an interstitial case you can see all the lattice sites are occupied with the host atom and the impurity atom is occupying the interstitial position. In case of substitutional it is occupying the it is taking the lattice site occupied by the host atom and that is why it is called substitutional defect or it is called substitutional impurity atom which is occupying this particular position.

In pentavalent and trivalent impurity where we do prepare a semiconductor when we dope silicon or germanium by either pentavalent or trivalent impurity they occupy this substitutional positions only. By doing that we prepare a semiconductor either p-type or n-type depending upon whether we are adding pentavalent or trivalent impurity atoms ok. So, this is one of the example where you will find a substitutional impurity occupying this occupying the regular lattice site.

Then, one of the very important type of defect which you will find is called dislocation and this is a linear defect or which will have one dimension ok. So, it has a dimension where the length of the dislocation will be a one dimension and there is no other dimension to that ok. So, this is called a linear defect because it has one single dimension.

Actually how people started thinking about this particular defects has a nice kind of a story around it. Because, when people were looking at this plastic deformation that how material deform they found out that the two atomic planes or two layer of atoms actually have a slip over a particular plane ok.

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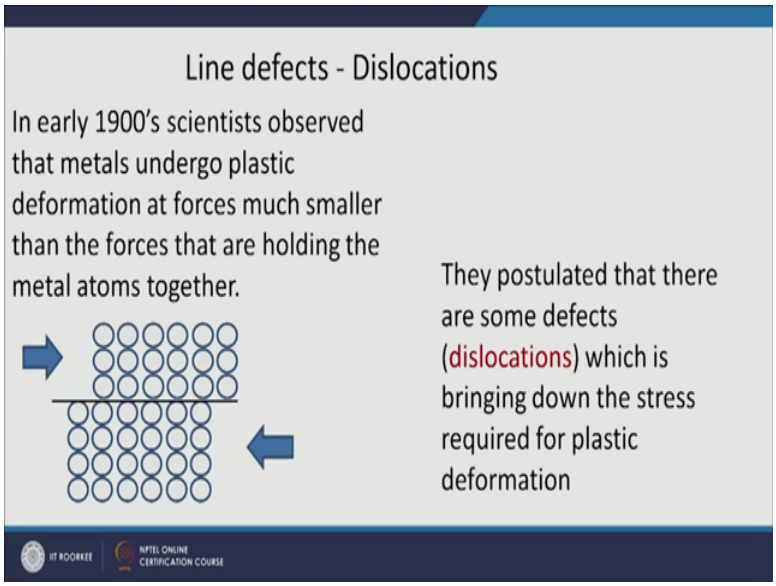

For example, I can show you this slide this animation here. So, you have arrangement of atoms and I have shown a plane with a black line here and I am applying the shear stress on this particular arrangement of atoms and because of that there is a sliding of atoms ok. So, upper half of atoms are sliding over lower half so, you can say see that in the previous arrangement there was some bond between all these atoms let me go back.

So, you have all the bonds between these two atoms and this will be along the whole plane and when I am applying the shear then all these bonds for all the atoms are going to break and they will form new bonds ok. So, all has to break and we have to find new bonds.

Now, the problem with this whole scene here is that we are simultaneously breaking all the bonds and creating this slide of atoms or this sliding of atoms and this is going to require hell lot of energy. So, the forces which people found out were much lower than what you will calculate by doing this kind of movement where all the atoms are taking part in the sliding process together the all bonds will be broken and new bonds will form and this it will require very high energy and very high force.

But, the measured force was much lower than that ok. So, then people thought or they postulated that there may be some defects in the material which is helping us to deform a material at a very low force or which require much lower energy and they they started

calling it as dislocations and the why this dislocation require less force I will show you in the next slide.

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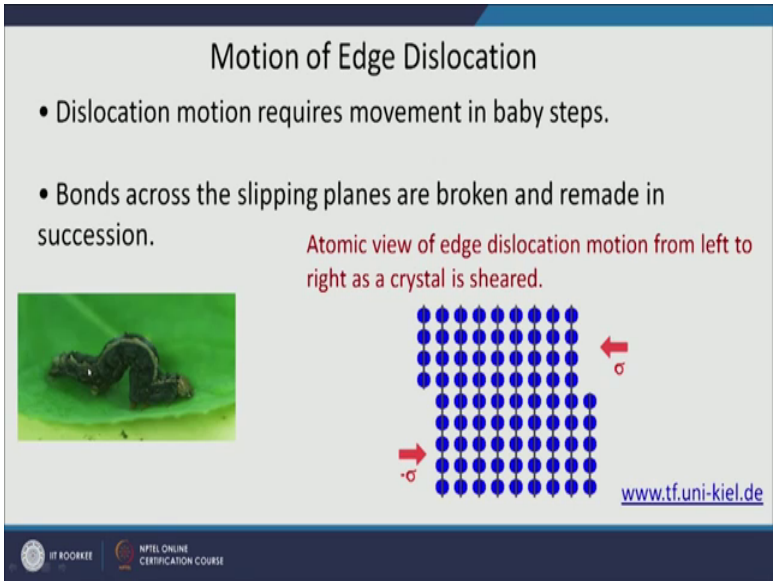

You can see a nice image of fear of a caterpillar how it is moving. So, a caterpillar will never move like this what it does it moves in a step like that ok. So, it raises it is body away from the earth and then it moves ok. So, that the idea is that it should have low very less friction or very less contact with the earth when it is moving and that is very nicely shown in this particular animation I have taken this animation from this particular website ok.

You can see that in each step one bond is broken. So, I am applying shear I suppose to the previous case where we broke all the bonds and created the step in this case you can see that when I am applying the shear stress here the bonds are broken one by one. So, you create this is and then you create the step at the end.

So, instead of one big step what we are doing we are moving or we are creating this step by small baby steps, one by one and this will give this will require much less force than what is required if I slide all the atoms together and this sliding is held by the creation of dislocation in the material. So, that you can see by a this red line here which is depicting the dislocation, which is helping and creating the step at the end, ok.

Now, of course, it was initially thought about that this type of idea is there and later on when electron microscopy was invented and transmission electron microscopes were developed then people saw that actually this is the case and you can see this is a nice micrograph.

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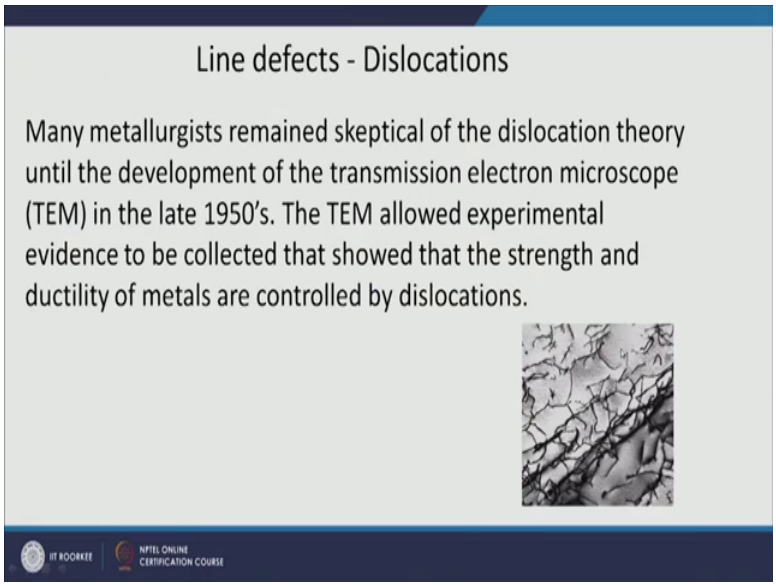

And, you can understand the actually the scale length is not there, but these are at nanometer scale and all these lines which you see are dislocations these are all dislocations and people did lot of experiments that if you do lot of deformation dislocation density increases. If you do any link this dislocation density goes down ok. So, by that you they could understand that this dislocations are the main source or main driving vehicle for deformation and that is what they and they control the strength and ductility of metals.

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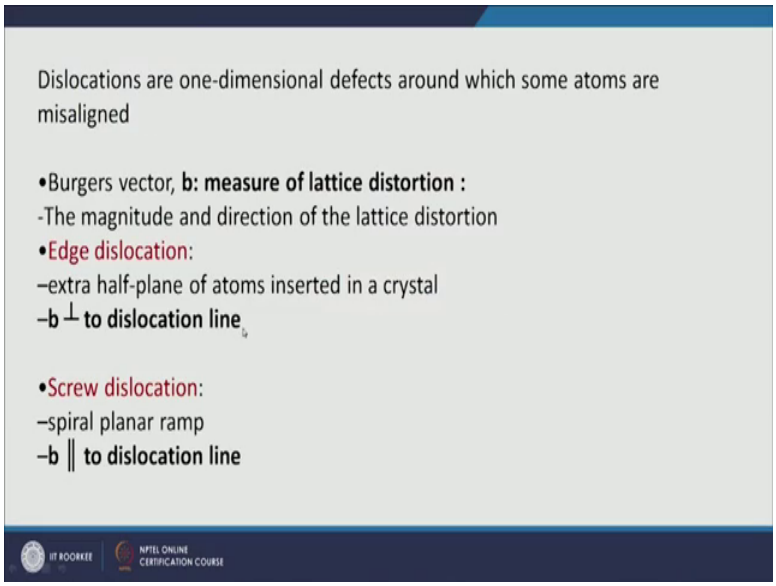

Now, I can divide this dislocation also in two, I can classify in them in two ways one is what we call as edge dislocation in case of edge dislocation the burger vector is perpendicular to dislocation line, we will see what do we mean by a burger vector and in the screw dislocation the burger vector is parallel to dislocation line. So, you can have these two type of dislocations and based on how the burger vector is with respect to the dislocation line ok.

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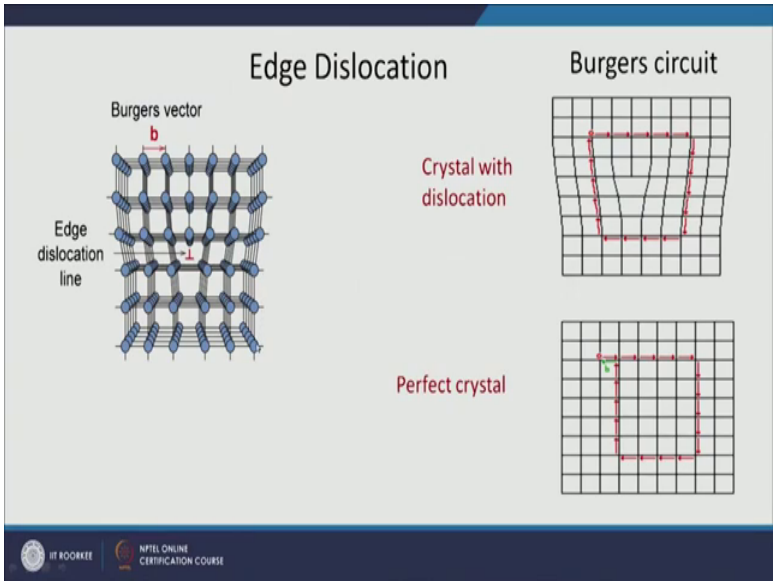

So, for example, here you can see a nice wire frame kind of structure ok. So, regular arrangement was there, but you have inserted a half plane in the arrangement ok. So, initially you can see that I have a simple arrangement like this maybe one more I can put here. Now, I have inserted another half plane in that. So, what will happen these suppose I have inserted up to this point then this atom will kind of give some space for this extra half plane and that is what is shown here.

So, wherever the dislocation is ending the you can see that there is large strain in the in the atoms between the there is a bond length is there and all these bond lengths are stretched ok. So, you have you are inserting this extra half plane here after certain distance you will see that all are still nicely arranged on both the side, but, where the dislocation is ending the there is large number of straining in the material and you can see that this dislocation is going in the direction of the projection here on the slide. So, this is the end of the dislocation and it is going in the material like this. If I want to do see you it on a 2 dimension it will look something like this ok.

Now, let me define that what do we mean by the burgers vector here ok. You can see that this one particular slide this one picture here has a dislocation a half plane ending here and the dislocation line is going inside the projection, this is a perfect crystal. So, we will take steps we will roam around the dislocation and see that how many steps are required ok. So, let us these we start from here 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14 15, 16, 17, 18, 19, 20 ok.

Now, same thing we will do here as we have done we are starting from the same position we are going along taking the same steps and we will find that we are reaching early here. So, extra step which we took here because of the extra half plane we are not going to take in the perfect crystal ok. So, this extra distance which we are traveling in the crystal which contains dislocation that is going to give me the burgers vector ok. So, this is my extra half extra length which I have traveled which is equal to this atomic spacing here and that is equal to b, that is the burgers vector.

So, by using burger vector I can define that what type of dislocation is this in a another plane the burger vector will be different because the atomic spacing will be different. So, this is how the edge dislocation will look like and this is how by drawing a circuit around

the dislocation and a perfect crystal I can find out that what will be the magnitude and the direction of burger vector will be.

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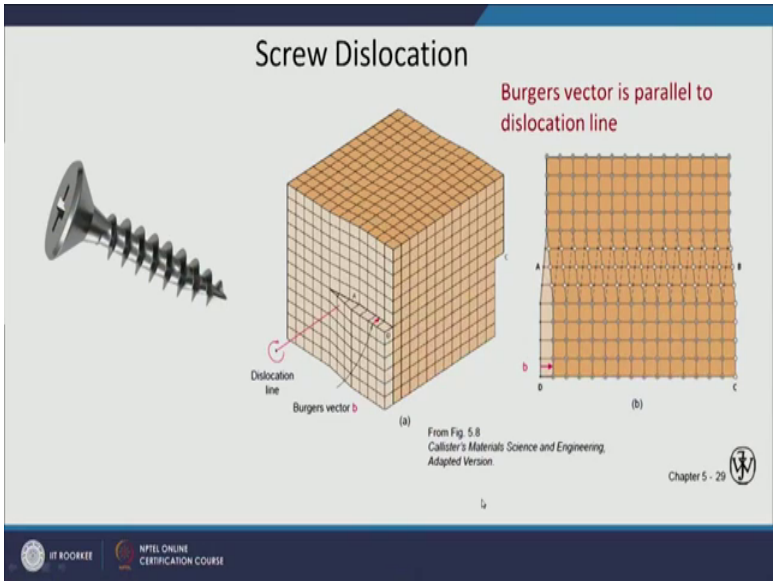

Similarly, in screw dislocation the actually the visualization is slightly difficult because it is a three dimensional movement of atoms around the dislocation ok. You can see it from a screw kind of geometry ok. So, if I am moving from this particular site and going along the screw ok, so, I will go down and then from the back I will come somewhere here ok.

So, when I am moving like this I have moved by a pitch of the screw as a mechanical engineer you will know that this is what we call as pitch of the screw. So, I have moved by a pitch of this screw in which in case of dislocation is the burgers vector. So, while I am taking this one rotation I have moved by one burger vector here and that is what is shown here that if I this is the open circle and the closed circle small the atoms are shown in the in the lower plane and the close open circle are shown on the upper plane ok. So, in these two locations they are one above another, but where the dislocation is they are displaced by a small distance. So, when you travel one whole distance you will create dislocation of one burger vector ok. So, this is what we call as screw dislocation. So, one is edge dislocation another is screw dislocation.

You do not have to worry about too much about this classification. Only thing we have to understand here is that dislocations are there in material and they help in the deformation process by doing this slip of two atomic planes by in the steps rather than in one step.

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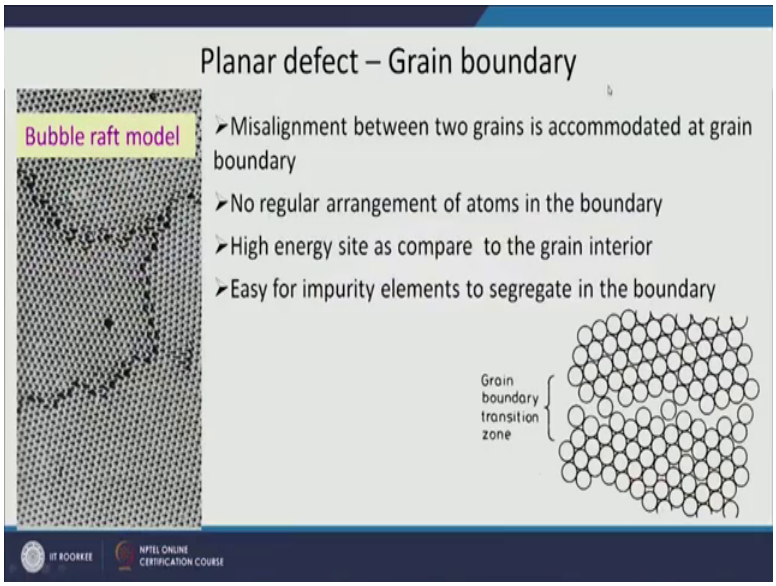

Then, the next one which is of importance already we have seen and we have discussed about grain boundaries. This is a planar defect means it is over an area. So, basically what grain boundary does is, it kind of accommodate the misalignment between two grains as you can see that there is a nice atomic arrangement here in one direction.

In another grain also you can see a very nice atomic arrangement is there, but where these two arrangements are meeting because their alignments are different I have to have some kind of an area where this misalignment can be accommodated and then the new alignment will start and that is what is called as boundary in this case it is because between two grains you call it as grain boundary. And, where you have grain boundary you can see that arrangement of atom is not regular as in the grains or as in the crystals and the bond lengths are also are not of equilibrium distance they are kind of stretched.

So, you can also understand that these are high energy areas because the bond length is not at their equilibrium distance and also you can see because there are more gaps available here. For any impurity atom or foreign atom to come and sit here is very easy for it ok. So, there is a segregation of atoms in the grain boundary. So, whenever you have foreign atoms sometime you are alloying make a making an alloy for those alloying element it is very easy for them to come and sit at the grain boundary which we which we usually do not want, but because there are large number of grapes gaps in the boundary that is the these atoms come then sit in this boundary sites ok.

A nice kind of analysis people have done about grain boundaries by this kind of bubble raft model. Bubble raft means these are soap bubbles which are arranged in a in a three dimensional area or space and those areas are photographed you can see that in these bubbles also some arrangement will be there will be a nice arrangement and suddenly somewhere there is the arrangement will break and the next arrangement will start.

So, you can see that this will be a nice arrangement it will look like a grain ok, but in this part there is another arrangement coming and this will be the boundary which is accommodating the misalignment between the two grains. One another an interesting thing you can see here is that there is a vacancy here, that means, one bubble is missing from this side. So, there is a vacancy also here.

Then, there are some special type of boundaries are also there which in this case one of the boundary which we have is called twin boundary. So, the twin boundary as the name suggests you can understand that it has a mirror kind of arrangement across the boundary ok.

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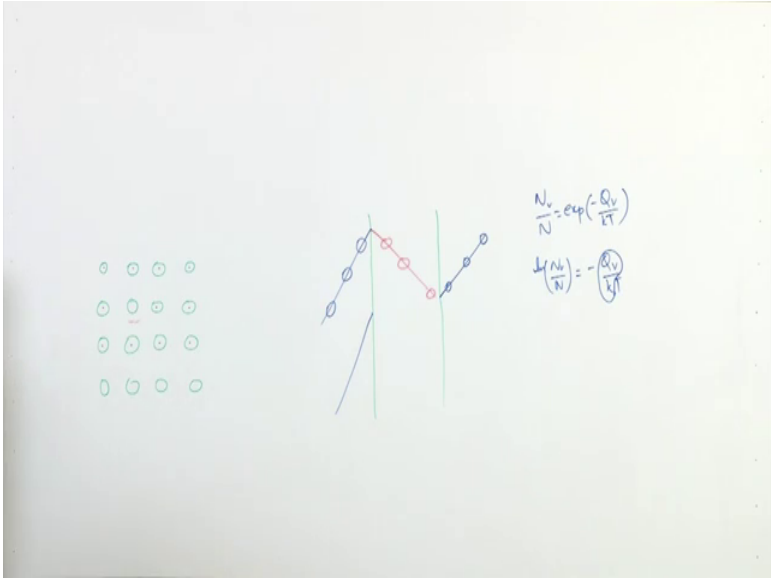

So, suppose in one grain the arrangement is like this ok. So, suppose this is my boundary and this is the for example, atoms are arranged like this. So, if you see this thing in mirror how you will see it? This atom will be mirrored here, this atom will be mirrored here, this atom will be mirrored here. So, it looks like that there is a mirror here and all these atoms are there is a reflection of this atom across the in the mirror and this kind of

boundaries are called twin boundaries which has a mirror like a arrangement of atoms across the boundary.

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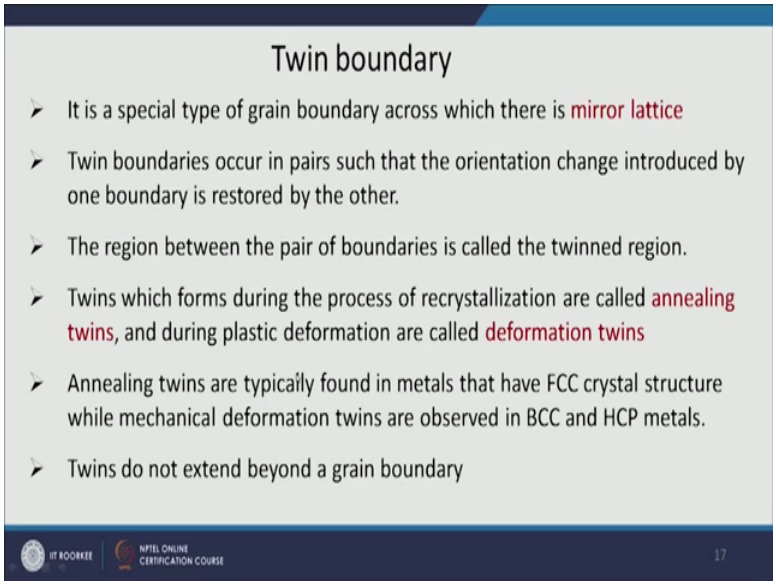

Some other properties of twin boundaries are that usually not always they occur in pairs. So, there will always be two boundaries together. So, whatever change in orientation is there. So, you can see that the this is this arrangement and then there is another type of arrangement. So, when another boundary comes it is a it will again become the same arrangement as this one.

For example, if I put another boundary here ok. So, across this it will again become the this will be reflected here, this will be reflected here, this will be reflected here. So, you can see the arrangement is again coming back to the original arrangement. So, if you have two boundaries together the orientation change introduced by one boundary is restored by the other. The region between the pair of boundaries is called the twin region. So, this area will be called the twinned region.

Twins which form during the process of recrystallization are called annealing twins and during plastic deformation are called deformation twins. Annealing twins are typically found in metals that have FCC crystal structure, while mechanical deformation twins are observed in BCC and HCP metals.

So, you can understand that all these features are also dependent on the crystal structure which we studied in the beginning twins do not extend beyond a grain boundary ok. So, a grain boundary will be the kind of a limiting for a any twin to go beyond that.

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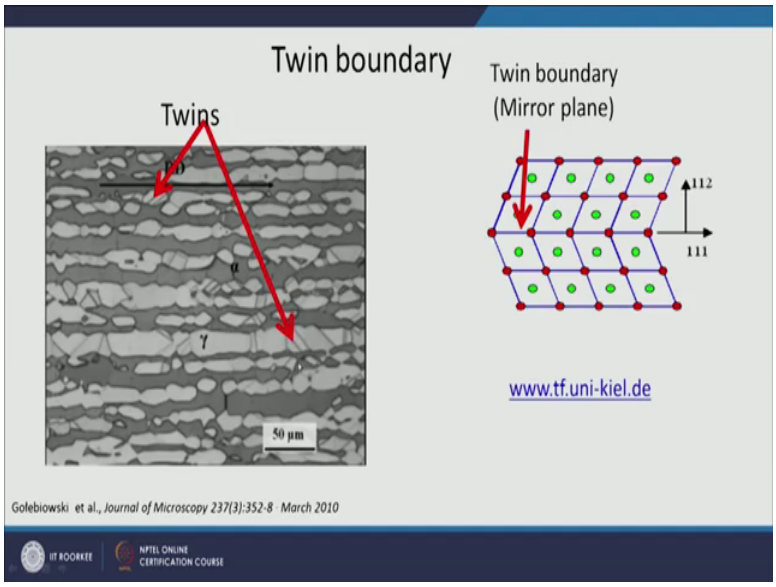

So, if you remember I showed you this kind of twins earlier also in the same micrograph. You can see that these two twins are coming in pair. There are other location also where the twins are coming in pairs; for example, here they are coming in pair and you can also see that they are not going beyond their particular grain. So, they are starting from here, ending here ok. So, it is not going beyond this particular grain boundary here., this also you can see because anyway there is another phase coming. So, it will not go beyond this particular phase boundary here. So, the phase boundary or the grain boundary will be the limiting where it will not go beyond that.

You can see the idea which I was telling you there this is my boundary and this particular atom is mirrored here, this one is mirrored here, this one is mirrored here and so on. So, it looks like a mirror boundary and the atoms on both the side look like any mirror image of each other ok. So, these are called twin boundaries. These are a special type of boundaries it will not be very commonly seen, but in certain situation it will be very prominent as you can see in this particular case. So, in alpha phase which is BCC crystal you would not see any twin, but gamma phase which is an FCC you are seeing lot of twins in the same material.

So, with that this is about defects ok. So, we have seen point defects, line defects and area defects. Line defects the dislocations are a very important defect to understand because lot of properties depend on them. Similarly, grain boundary is a very important defect because grain boundary actually limits the how that how much the dislocation is going to move which we will see later on also ok. So, defects is very important to understand and we will use idea of this defects later on to understand a lot of structure property correlation, ok.

Thank you.