Solid State Chemistry
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Lecture – 33
Line, Planar and bulk defects in crystals

Now, I will start with the 3rd lecture of week 7 of this course in this lecture. I will talk about other kinds of defects; we have already seen point defects in the last lecture in. Now, I will talk in a little bit more detail about the other kinds of defect in particular line defects and planar defects.

So, week 7, lecture 3 will be on Line, Planar and bulk defects in crystals. And again let me emphasize that I will talk very briefly about these topics and I encourage you to look at for a better understanding, you should look at other sources.

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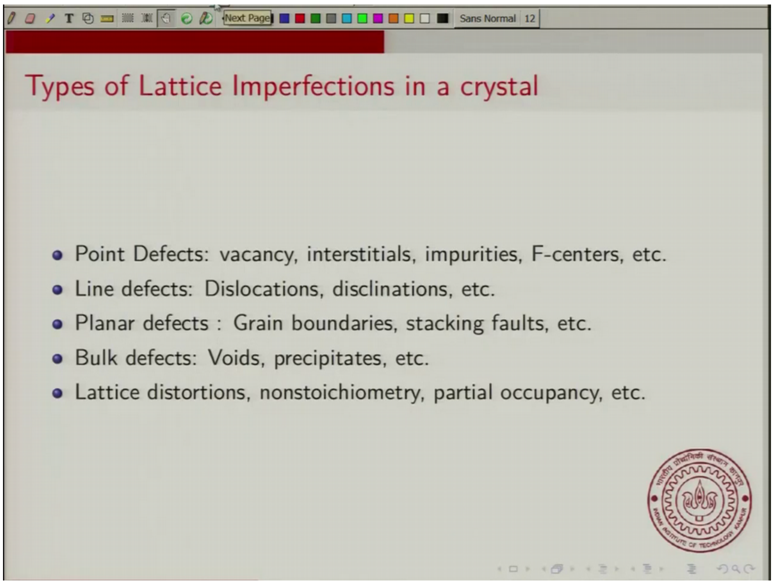

So, just to recall we talked about different types of lattice imperfections in crystals. So, you could have point effects such as vacancies interstitials impurities and F centers which we which we briefly looked at in the last class.

Then there are line defects which are which we look at today disclinations and dislocations. Then there are planar defects bulk defects and other lattice distortions are also possible I will talk about line defects planar defects and bulk defects in this class. So, the first kind of line defect I will talk about is called an edge dislocation, this is a kind of a dislocation and I will talk about this, because it is relatively easy to explain, ok.

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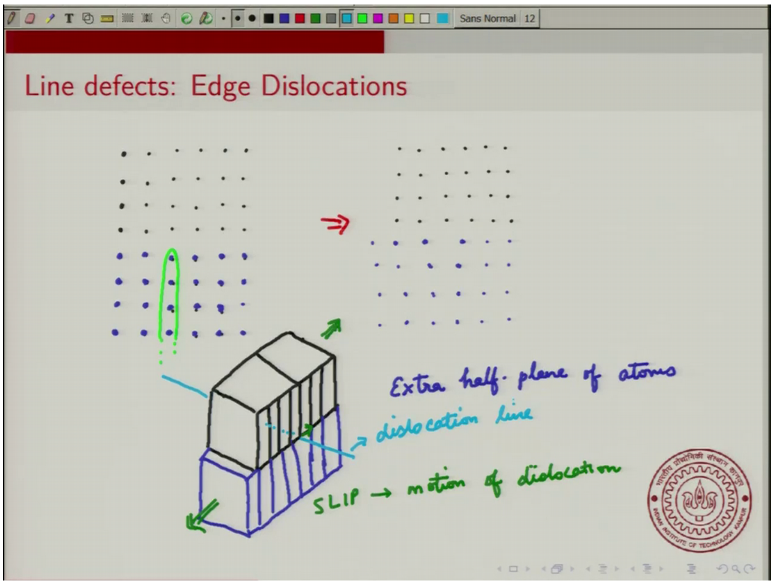

So, now imagine that you are looking at a cross section of a crystal. And imagine that these the atoms of the crystal, have some regular arrangement. And I am just showing some regular arrangement and you do not need to I am just showing a cross section. So, it just looks two dimensions, but it is really part of a 3 dimensional crystal and imagine that this is a perfect crystal.

So, this is a perfect crystal with atoms located at the lattice sites. Now let us imagine that we, that we do the following we take out half a plane of atoms, ok. And let me, let me just show it in a different color. Let us say, you take out all these atoms that have enclosed in green. And, we imagine that we do it all the way to the since the crystal extends, you take it all the way to the end of the crystal. And I call this a plane, because this is actually I here, here it just looks like a line of atoms, ok, but, you should really imagine that the crystal is extending all the way outside the screen outside the screen.

So, it is really a plane in if you, if you take all the atoms going, gdirectly out of the screen in this screen, you will get a plane of atoms. Now, imagine that you just take out those plane of atoms, ok. And then what you do is now you rejoin the crystal, ok. So, you rejoin the crystal so, that away from that plane of atoms everything looks the same. So, these are the atoms about both the plane. And let me just for convenience let me show these, these atoms in blue color, ok.

So, above the plane you have all the black atoms and I am just this is just a cartoon representation. So, it is not it is not going to be exactly correct, but it will give you the basic picture of this dislocation. Now you have the blue atoms and you have one blue atom missing here, ok. And, because it is missing we will just say that these atoms will come a little closer. And they will and I will just show how I will show what kind of things you can.

Now you get now, you see what I have done, ok. So, so you had this missing plane of atoms I took this out and then and then in order to fit the atoms I moved all these atoms towards this side move these atoms a little bit towards this side, ok. And right, right at this point I just, showed the amazing atom, but you see that all the atoms near it have actually moved a little bit, ok.

And now what we did if now if you put this extra plane, you will see something like this, ok. So, if you put the same number of atoms, you will see something like this, ok. So, this is that plane of this is a half plane of atoms that we had taken out, ok. So, we take out a half plane of atoms and then you rejoin the crystal, ok. So, this is called an edge dislocation, ok. And I will show another picture which will be, which will be more in the, context of the, the 3 D, 3 dimensional picture of this edge dislocation, ok. And let me again use the same colors black to show the part where there is not been a not been a dislocation.

So, I am just showing part of the piece of the crystal, ok. So, this is a piece of a crystal and this is the sort of the perfect part of the crystal. And what I imagine is that below I have the piece of the crystal where I removed one plane of atoms, here one, one whole plane of atoms in the crystal and then I after rejoining, ok. So, what it looks like is, ok.

So, we so, you can imagine you can see that this black plane of atoms, ok. It extends only up to here and in this side, it removed and all the other planes extend all the way, ok. And now that extra plane I will show it here, ok. And this is actually quite relevant to the crystal, ok.

So, this emphasizes that there is an extra plane of atoms, that is due to this edge dislocation, ok. The other thing that is emphasized by this is that when it comes to the surface, ok. There is an extra plane of atoms so, , there will be this kind of step feature on the surface, ok. So, this edge dislocation has an extra plane of atoms, extra it is actually a half plane of atoms, I use the term half plane is used, because you are taking only, only half of these atoms. And really it is a whole, it is a whole plane of atoms that goes all the way, all the way inside, ok. It goes all the way through the crystal.

So, here we are only seeing a cross section, but the plane of atoms goes all the way through the, through the crystal, ok, it is, half plane of atoms. Now there is a very important connection between the mechanical properties of the crystal and the presence of dislocations. Now if you, apply a shear stress on the dislocation, a shear stress means here you can think of it as applying a, applying a force in this direction and a force in this direction, ok. So, that will be the, the shear stress on the, crystal, ok. Then this extra half plane of atoms, can actually move, ok. So, so then this missing set of atoms that are right here, that can move, ok. So, it can this, this row of atoms can move here; then the then the missing plane comes here.

This behavior is called slip behavior slip this relates to the motion of the dislocation. And what will happen when you do this is that this dislocation will move along this direction, ok. This dislocation will move this, ok. Now, the dislocation is not is not just here actually the dislocation corresponds to a line that goes all the way through the crystal, ok. So, this the, it is a the dislocation is characterized by this line which is referred to as a dislocation line and this dislocation line is a it actually goes this way, ok. So, it is going, it is going through the through the, through the crystal and ok.

So, you have to really imagine that the crystal is infinite and this is your dislocation line. And if it is, a perfect edge dislocation, it will just be a straight line, ok. It will be a straight line and we will only terminate at the surface of the of the crystal, ok. So, it is a straight line for a perfect edge dislocation. Now the other kind of dislocation that is very common in materials is a screw dislocation.

So, screw dislocations can be visualized, they are, also a kind of line defect and it is easy to visualize them when you, when you think about, if you, think in the following way, ok.

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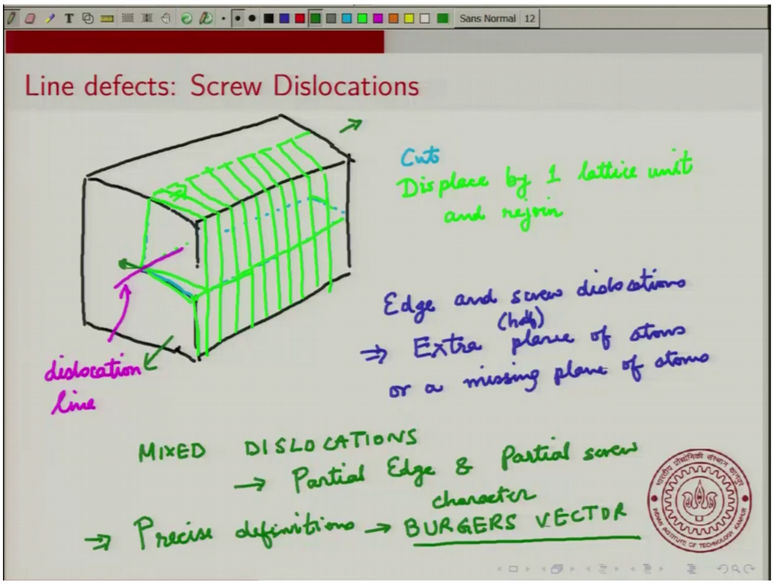

We you, you imagine that you have a, perfect crystal, ok. And what you imagine is you, imagine that you break this crystal, ok. You cut this crystal along so, if you have a perfect piece of crystal. Again, I will show the same kind of picture that we saw in the in the discussion on the edge dislocation.

Now, now what you imagine is you take this perfect crystal and you break it, ok. So, you cut it this way, cut it along here and, and imagine that you cut it all the way across. So, so it goes. So, you imagine that you cut it in this way.

So, you just make a cut in the crystal, ok. And you can see that I am cutting it only half way into the crystal I am not cutting it all the way through I am not going all the way to the other end of the of the crystal, ok.

So, you imagine making this cut, ok. So, you just make a cut, then what you do after that is you, you imagine taking this top half of the crystal, ok. Just let me, just extend this and you just displace it, ok. So, you displace it in this direction let me use a different color. So, , that is displace by one lattice unit, ok. And now after you displace by one lattice unit then these the, the new what you will see is that you will see it going like this, you will see these atoms coming like this and going like this, ok. So, you made the cut here and after you displace then these atoms will come this way, ok.

Now, after the displacement you can see that this row of atoms looks like this. So, what you have done after displace by one lattice unit and you have rejoined it and rejoined, ok. So, after you do that what you will find is, you will find that this hole, you will have you will have something like this, ok. Now, now what is to be noticed is that is that the dislocation line in this case, ok. So, this is the dislocation line, this is the dislocation line, ok. And what you also see is that now when you shear the crystal when you do the same, same thing that we said in the last time you apply forces this way in the crystal, ok. You shear it then what then this dislocation will actually move in this direction.

So, the motion of the dislocation will actually be in this direction. So, you really have to imagine that when you take this when you take this dislocation and start sharing it. Then what will happen is that is that the direction of slip and the direction of motion will be this way. So, instead of joining here, it will join here, ok. And you will like you will get, you can imagine that you will get a longer this curved line will be longer, ok.

So, the screw dislocation is another kind of dislocation and both edge. And screw dislocations, they can be visualized as extra or missing plane of atoms, you can think of it as an extra plane of atoms or a missing plane of atom. And extra and I should, I should, I should emphasize that it is really a half plane, ok. So, these are really half planes, ok.

Now, now both these locations, ok; there are ways to actually characterize these dislocations, ok. I will not get into that here, ok. What I do want to say is that, is that you can have, you can have what are called as mixed dislocations, where basically the dislocation has partial edge. And partial screw, screw character, ok. And you can actually formerly you can, you can you can give a very precise meaning to this, ok.

So, there is a precise definition which, which I will not talk about, ok. So, I will just, but I will just write it here. So, there is a precise definition, this is based on the idea of a Burgers Vector, ok. So, and this will not be done in this lecture, or in this course we will not be doing this, ok. So, let me emphasize that I will not be talking about Burgers Vectors, but for those who are interested, you can look how do you characterize a dislocation using this concept of a Burgers Vector, ok.

There is another kind of line defect which is which is less commonly known which is called a disclination, ok. So, here there is a change in orientation.

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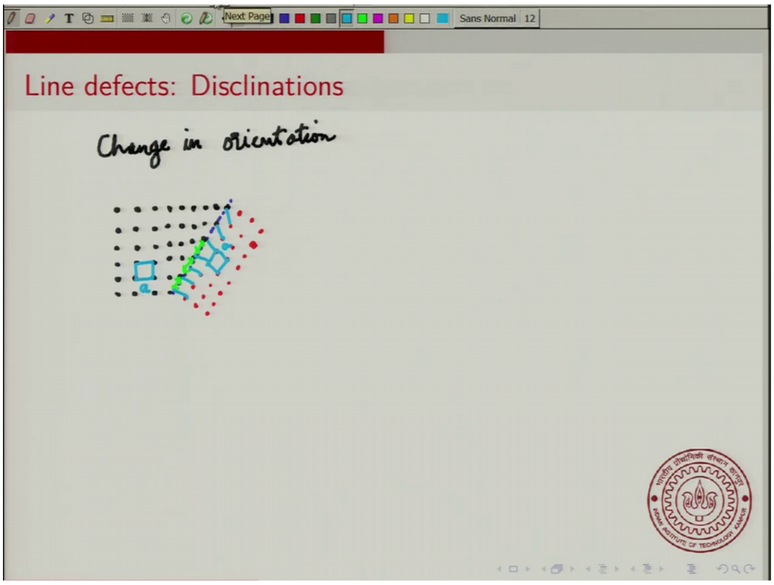

So, this refers to a change in orientation, ok. So, you can think of it this way if you, if you have for example, if you have, I will just, I will just show it in two dimensions; if you have a, if you have a crystal that looks like this perfect square lattice.

Now, let me imagine that I have a line here, and let me show it at some at some tilt and so you are. So, a crystal to one side of this line is oriented in this way, ok. Now, to the other side of the line the orientation changes, ok. And let us say that the crystal is again, again the same lattice, but at a different orientation. So, for example, you could have, you could have something like. So, it is the same structure, but it had a different orientation, ok. Then this would be, this would be called a disclination, ok. So, such a, defect is referred to as a disclination.

Again, again it is what is very crucial to remember is that this lattice constant and this lattice constant are the same, ok. It is the same lattice, ok. It is just that the orientation is changed, ok. So, it is just a change in the orientation across this line. Then this line is referred to as a disclination line, ok. So, disclinations have now, notice that if you look at these distances, these distances will, actually be larger than the lattice spacing.

So, if this lattice spacing is a then this the spacing between atoms on this line will actually be greater than a, ok. So, but, in this crystal, ok. These again are this spacing is again a, ok. So, there has to be some matching of there has to be some matching of these atoms here, and that is what leads to this disclination, ok.

So, disclinations and dislocations are the kind of are the most common line defects that you have ok, but you can also have, you can also have other defects. Now lined effects have a very important consequence on the mechanical properties of crystals, ok.

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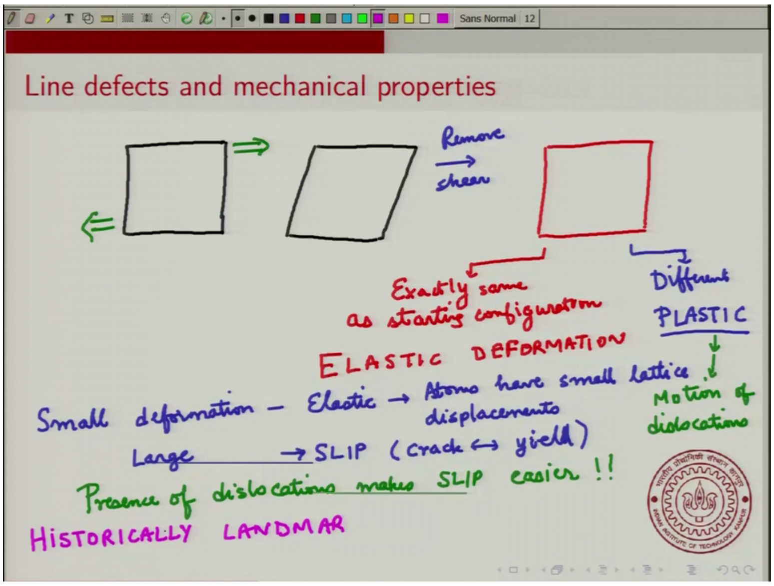

So, what we saw is that when you if you take a crystal. And you imagine that you are, you are, you are, taking this crystal and you are sharing it. So, sharing it you can I will just, I will just show it this way that you this is imagine that this is a three dimensional crystal and you, apply a shear force, ok. So, shear force means you apply one force and this direction and one force in this direction equal and equal and opposite, ok. And what this will do is it will tend to deform the crystal, it will tend to cause the crystal to be deformed, ok.

And now, , so the question is how if you, now take out this shear, ok. So, now, now if you remove the shear, so, you remove shear, ok. Then does the crystal come back to exactly the initial configuration, ok. So, does it come back to if you remove it, it may there are two possibilities, ok. So, either this is exactly the same as exactly same as starting configuration, ok; that means, that means it is exactly same as this configuration, ok.

So, , if this so, you do a shear and then you remove the shear and then if it comes back exactly to what it started with, ok. Then we refer to this as elastic, elastic deformation and the other case when it is different from the different then we call it a plastic deformation, ok.

So, if, this configuration, after you remove the shearer is not the same as what you started with, then we say that the crystal has undergone a plastic deformation, ok. And typically most crystals, will behave elastically for small deformation, ok.

So, , small deformations is usually elastic, ok. In this case, the atoms just move a little bit from their lattice positions and then they return to. So, atoms have small lattice displacements ok; that means, they are very close to where they were in the lattice, but just small displacement of atoms, ok. So, this refers to the elastic deformation.

Now, if you have a, if you make the deformation too large, then the atoms will actually, actually slip this is actually a crack, or, the mechanical term is yield, ok. So, for larger deformations so, when the deformation is too large then there will be a slip it will crack or yield, ok. So, if you have a perfect crystal, if you if you have a perfect crystal then this is what you can expect, ok.

Now, now if there are dislocations so, presence of dislocations makes slip easier, ok. So, if your crystal has these dislocations then it is actually easier to do this slip and this larger deformations in this. So, plastic deformation and plastic deformation becomes easier, ok. So, plastic deformations are related to dislocation motion, ok.

So, this is really related to motion of dislocations and you can see that when you move a when you when you apply shear let us just go back to the previous slide where we showed the plastic deformation, ok. So, when you apply this plastic deformation this dislocation will move, and once it moves if you take out this deformation the dislocation is not going to move back, ok.

So, these are permanent deformations in the material, ok. So, so the presence of dislocations actually makes slip a lot easier, ok. And this is very- very, it is historically a very important observation, that this was historically, it is a landmark observation, it is a landmark observation.

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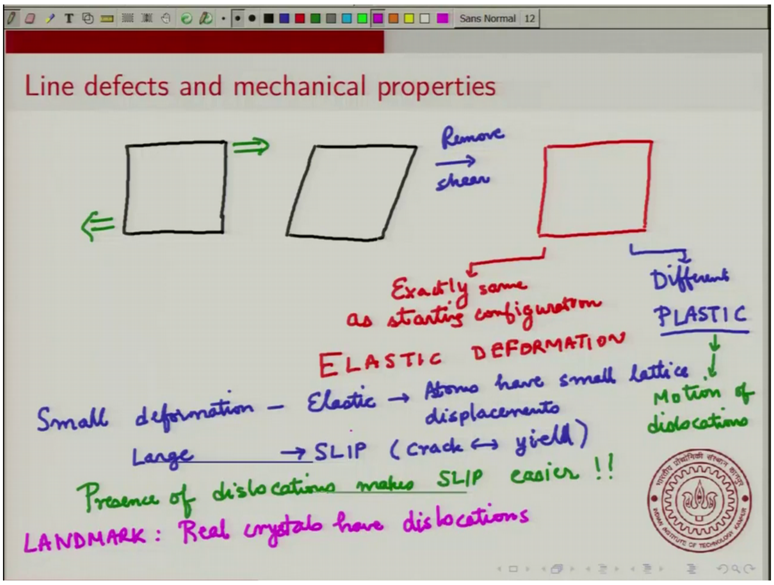

Note we will just say it sure, It is a landmark observation which so, real crystals have dislocations. So, what I mean is that the, the theoretically calculated the strength of a crystal, ok. It was much larger than what was experimentally observed. And therefore, people concluded that real crystals have dislocations, ok. And this and this basically had to do with a chemical experiments where they checked at what shear stress the crystal starts showing, showing yield or large deformation.

So, when does it start slipping, and clearly if you had a crystal with more dislocations, it would slip easier, ok. Then a crystal without any dislocations,ok and so, , when the real when the properties of crystals were seen, it was observed that the theoretically calculated strength was much larger. And when I say much larger, it is like you know from about 10 raise to 4 times larger than what was photo seen experimentally, ok.

So, therefore, it was concluded that it, it was actually postulated that real crystals should have these, these line defects and, and then soon enough they were actually observed in real crystals. So, again, I mentioned briefly about elasticity and plasticity, ok.

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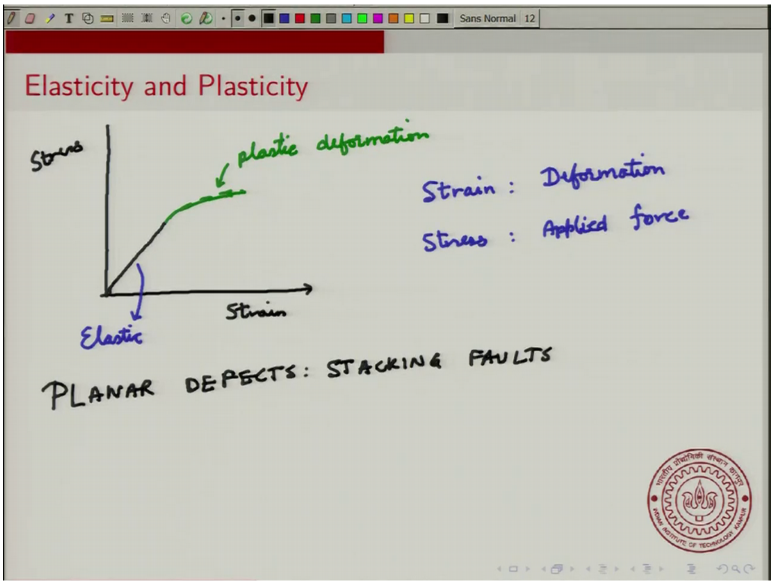

So, what we say is you can show this in some sort of a graph, ok. What is typically shown is something like a stress was a strain curve, and strain was a stress.

So, if you take any typical material, stress and strain are proportional to each other. This is this is the linear elastic regime. And at some point, at some point the crystal will start undergoing plastic deformation, and when it undergoes plastic deformation so, in this elastic region, if you take out the stress, it will come back to it will come back to the unstrained configuration and this is the plastic deformation, ok.

You can, have you can have other behaviors also for the typical behavior will have an elastic region and a plastic region, ok. And now I should emphasize that, that strain refers to deformation; that means, how much you can deform the crystal deformation, ok. And stress refers to the applied force, ok. Formerly it is the, it is related to the applied force per unit area, ok. And in strain is related to the deformation per unit length ok, but I want, I want, I just want to emphasize that strain is related to deformation stress is related to the applied force, ok.

So, once it starts plastically deforming a very small increase in applied force can lead to a large change in strength. Now, let me let me also briefly mention some other type of defects that are possible, ok.

So, I will talk about I will talk about planar defects such as stacking faults. Now, so, stacking faults and grain boundaries are kind of planar defects and I will just illustrate the idea of a stacking fault using the idea of a cubic close packed.

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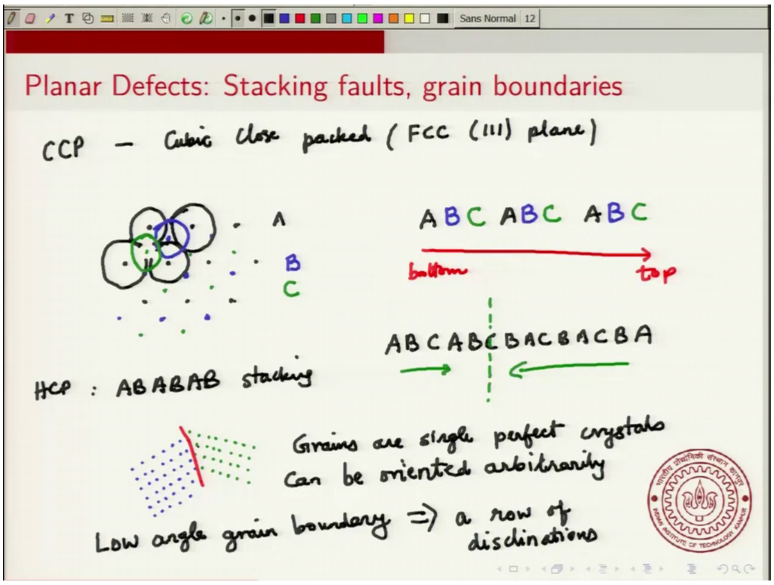

So, cubic close pack structure, and you can, think of this as the, as the one, one direction of the of an FCC. So, that is a cubic close pack structure. So, in this you can, you can think of this as in the following way you can, imagine that there is a there is a hexagonal lattice, ok. So, this is the z equal to zero layer.

Let me mention here that this is FCC and as it is actually the 111 miller plane, ok. I have not explicitly discussed inhaler planes, but we will see that, ok. So, this is the first layer this is z equal to 0. And then the next layer, is located here or let me call this layer a. And the next layer is right at the centroid of these triangles at the centroid of these triangles and this is called the B layer,ok. And that, that you assume I mean you can, you can really think of these as, as spheres, that are touching each other.

So, if you, if you imagine that one sphere is like this and another these three spheres from a pack in this manner, ok. And the next layer is right in this region, ok. So, that is the B layer, and the C layer, ok. In this cubic close packed there is a C layer which is actually in these positions, these positions, ok. It is in the, , it is a centroid of the other triangles.

So, this is the standard cubic close packed structure, and so, so the C would be something like this, ok. And so, this cubic close packed structure, it looks like, it looks like A BC ABC ABC let me write the BC B, ok. So, this is the, as you go from the from the bottom to the top. So, in this direction, you are going from the bottom to the top or vice versa you can go the other way also, ok.

So, it is referred to as an ABC ABC type stacking, ok. And now you can see what what kind of stacking fault can be there and to understand the stacking faults, we will just look at these at this at this part, where we show the ABC ABC, ok. So, a stacking fault could be something like this. So, so you can, you have A B C A B C, ok. And then what you have is here you have CBA, ok. In the sense you have the ABC ABC stacking, but in the opposite direction, in this direction.

So, here the ABC was in this direction here the ABC is in this direction and right at their boundary, you have a stacking fault. So, this would be a stacking fault, ok. So, right here, you have a change in the orientation of the crystal. So, on one side you see it is going in this direction and the other side the ABC is stacking in this direction, and you have the stacking fault here.

So, this is a very classic stacking fault. Similarly, for the hexagonal, hexagonal close packed hexagonal close packed is also a close packed structure. So, HCP has A B A B A B stacking, ok. So, it has A B A B A B stacking. Now in this case, you cannot really have a stacking fault, ok, you cannot, have I mean you cannot really have a, have a, have a change in the direction, because,, I mean A and B alternate each other ok, but when you have ABC ABC, you can have a change in direction, ok.

So, the stacking direction of this side of the crystal is different from the stacking direction of this side of the crystal, ok. This is possible in structures like cubic closed packed or more complicated structures and this is a planar defect, because, because actually this extends through this whole layer, ok. I mean this is an ABC, ABC actually represent a, a represents one whole layer. Similarly, B represents one whole plane of atoms, C also represents a whole plane of atoms, ok.

So,ABC actually represents a whole layer. So, this is actually the stacking fault is a planar defect, it is a whole plane of defective atoms, ok. So, the other example of a planar defect and I will not talk too much about this is a grain boundary, grain boundary is where the, where the, crystal is essentially growing in a different direction, ok. And you can have I mean the, you, you can have one grain of the crystal this way. And, and you could have let us say another grain of the crystal that is let me, let me just show it growing in some other direction, just to, illustrate the point and then that will join them well they.

So, I am just showing two crystals that are growing in two different directions, ok. They are the same crystal, you have to imagine that they are the same crystal and this would be a grain boundary, ok. So, you have in this grain is growing in this direction, this grain is growing in this direction, ok. Now, the grain boundaries are actually they can be arbitrary directions, ok. So, grains are single perfect crystals, ok. And you know this you know, you know grains can be oriented arbitrary, ok. So, they can be oriented arbitrarily, ok. And I will just make this statement, again you can, you can look up for more information, because I want I will not be talking about this more, ok.

But a low angle grain boundary, can be viewed as a is equivalent to a row of disclinations remember a disclination is a line defect, ok. Whereas, a grain boundary this is a planar defect, ok. And a low angle grain boundary can actually be viewed as a row of disclinations, again I will not talk too much about this ok, but this is some you some information that you might find useful, ok.

So, that is how much I want to say about planar defects. Now I will just say very briefly about bulk defects and again I am going to be very brief, ok. And now the two kinds of defects are I will talk about our voids and precipitates, ok.

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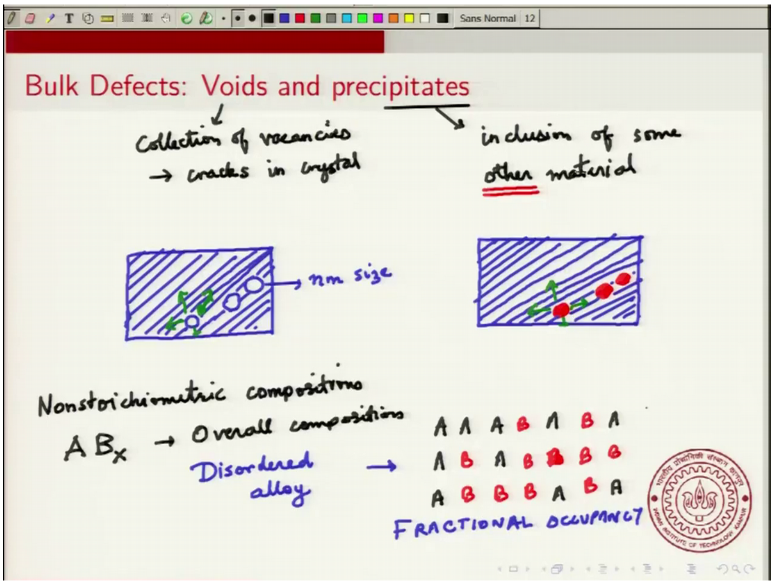

And a void is basically a collection of vacancies, ok. So, if you have a large cluster of vacancies, come together you form a void, ok. And you can this can also lead to cracks in the crystal, ok. And a precipitate is inclusion of some other material you can also have I mean inclusion of some other material. And let me put, let me underline the word other, it need not be a different material altogether, it could just be a material that is treated differently, ok.

So, for example, you could heat one part of the material, ok. And now that part of the material is hotter than the others, ok. And that would be an, that would be an inclusion or a precipitate. So, if you, look at a crystal, the voids in the crystal would be like these regions where there is no where there is no crystal, ok. So, if all this is the crystal, all this is a region of the crystal then the voids would typically look like this.

So, that is a fairly large, ok. So, so what should be kept in mind is that compared to an individual vacancy, vacancy refers to one missing atom, whereas, a void is a very large collection of atoms. So, typically voids are large of the outer of you know nanometers and more, ok. So, nanometer size and then inclusion would look let me take the, let me take the very similar configuration.

So, you have the perfect crystal all around, but somewhere you have some inclusion of some other material, ok. Now, in these two figures, you can see what will happen now whether you have a void or an inclusion, ok. The crystal the remaining part of the crystal will experience some forces on it, and more precisely it will, it will experience certain strains on it, ok. So, either due to the void or the inclusion either there will be some, some sort of forces on it, some sort of forces on the surrounding crystal due to the voids and the inclusion, ok.

And what is to be noted is that the voids and the precipitates will have very different effects, I mean there the, forces due to a precipitate will be very different than due to a void, ok. And these forces will depend on the precipitate also, and so, the mechanical properties of the crystal are greatly affected by the presence of voids and precipitates, ok.

And, so, this basically concludes the discussion on the line defects planar defects and bulk defects, I will just mention one more one more small point, ok. And this actually refers to refers to non - stoichiometric metric compositions, ok. And all I am saying is that is, that if you have a crystal, let us say of the form A B X, ok. So, this is overall composition and now let us, say let us say A and B are very similar in size let us say A and B a very similar in size, ok. So, and let us say they form a very almost, almost, their lattices are identical, ok.

So, , then your crystal would look like would look like you know some A, A, A and some handsome BS, ok. And what you can see now is that is that this is a completely disordered this is an example of a disordered solid solution. So, this is a disordered solid solution or a disordered alloy, ok. So, what you mean is that A and B there is no order. So, each site is either occupied by A or B, ok. So, so each site is either occupied by A or B and such that the overall fraction is so, overall composition is a times b to the X, ok.

So, here is a case of a crystal which is characterized by a fractional occupancy, ok. So, this has the concept of fractional occupancy, ok. And again, again this is something that we will see when we are discussing alloys more, ok. When we are discussing alloys and solid solutions, but you can imagine that instead of this you could, you could have A and B formed form a very regular, regular pattern, where instead of forming this fractional occupancy kind of structure, you could, you could have something like a regular structure like the zinc blende or, the sodium chloride or the cesium chloride, ok. Those are not fractional occupancy compounds, ok.

Those are regular compounds ok, but this is an example of A of a crystal which is characterized by this fractional occupancy, ok. So, I will conclude this lecture and with this I will conclude the discussion on the line planar and bulk defects. In the next lecture, we look a little bit at the thermodynamics of defect formation.

Thank you.