An Introduction to Materials: Nature and Properties
(Part 1: Structure of Materials)
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Lecture – 38
Defects in Solids (Point Defects)

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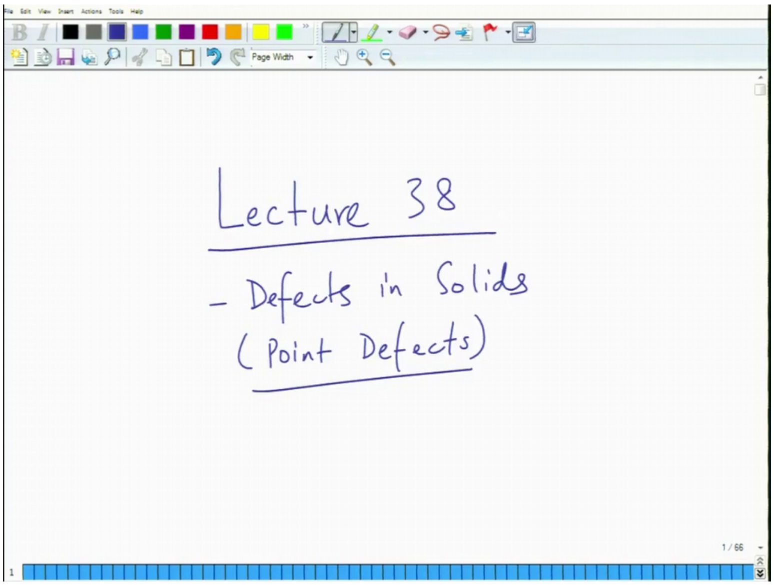

Ok

so, we now begin with lecture number 38 which is on defects in solids. So, this is the concluding part of our course where we last so, these three last lectures will conclude this course on structure and materials. So, what we have learned so far is about the crystal structures, the lattices, the structure of metals, the structure of alloys, the structure of covalent material, structure of ceramics, structures of polymers and glasses and finally, we looked at the structures or structure determination of materials using x ray diffraction.

And then, but so, far we have assumed that the structures are perfect ok; but structures are not perfect unlike like everything else around us. There are imperfections in crystals, which is what we are going to talk about in these next three lectures.

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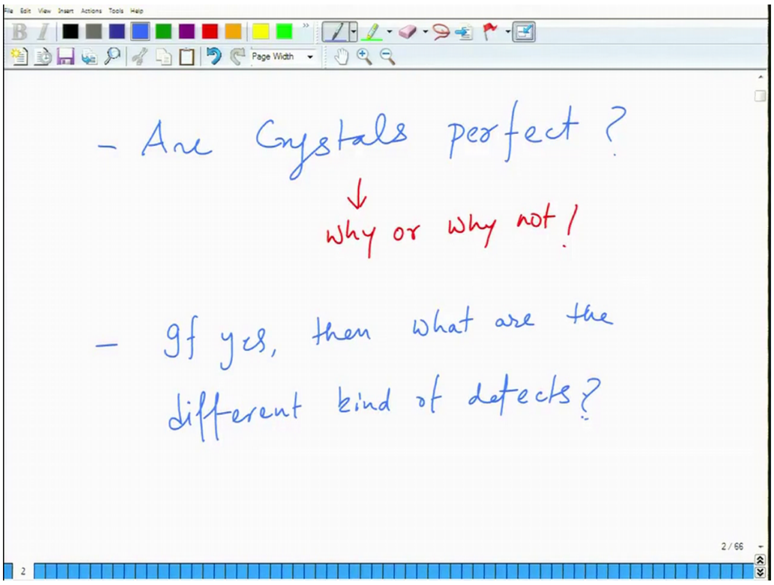

So, the question is first question is, Are Crystals Perfect? And the second question that we answer is if they are not perfect, if they are perfect then the answer to this question would be why ok; why or why not and then we have if yes then what are the different kind of.

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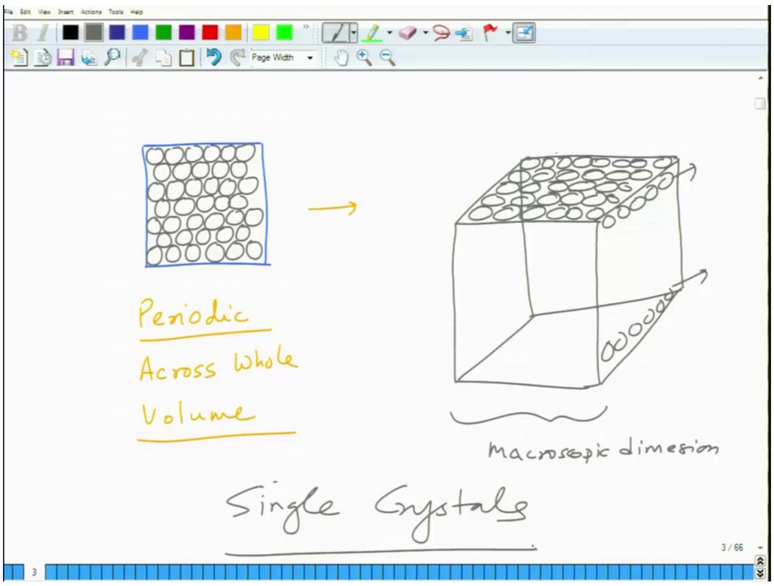

So, let us first begin with the first question are the crystals perfect well. Let us first before we talk about the defects, let us first look at the atomic arrangement in a perfect material. So, let us say we have a material in which atoms are arranged in this fashion ok, all right. So, this is basically we can say it is periodic, it is a periodic structure. But it is periodic across whole volume of the material.

So, whether it is 1 nanometer, whether it is whether it is 10 nanometer, whether it is 100 nanometer, whether it is 1 millimeter or whether it is 10 millimeter or 1 meter wherever you look atomic arrangement looks the same. So, if it is a layer and it is a layer all throughout that surface of the material ok; there is no other orientation that is present.

So, if you look at such crystals are called as, so if you if you draw such crystal; for example, a crystal might be this. This is your crystal. The dimensions are so, these are macroscopic dimensions and on the faces of the crystal the atomic arrangement is same everywhere.

So, if it is this here, if it is this here, whether you look here or here it is same there ok. So, atomic arrangement on this surface is same, all throughout similarly on this surface ok. So, this is called a single crystal; there is no discontinuity in the arrangement of atoms they it is uniform all throughout the crystal; this is called a single crystal ok. So, these are called as single crystals.

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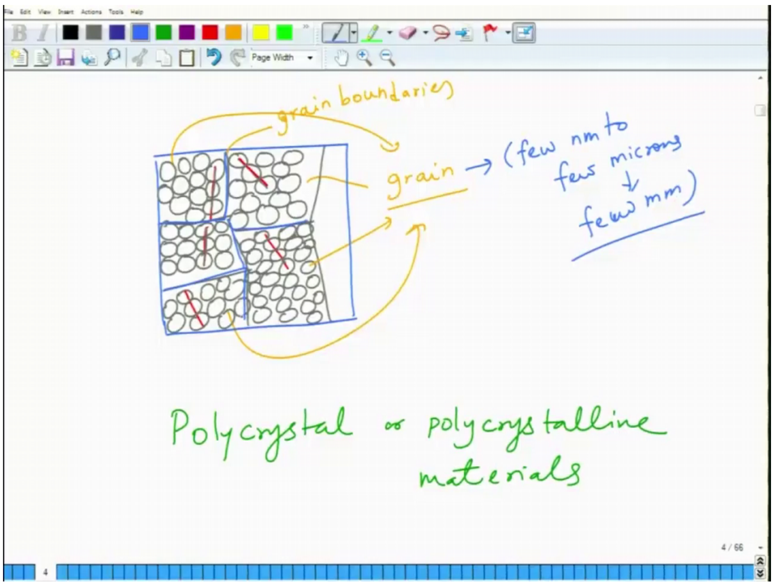

Now, life is not very kind to us in most occasions. What happens in reality in many cases in most cases is that materials are like this. You have enclosed volume like this. Within one volume you may have arrangement of atoms in this fashion ok. The next volume it could be something like this and in the next one it could be so, you can see that there is a distinct change in orientation here right.

This is a different direction and this is a different direction and this is a different direction. You can see that there is a distinct or change in the orientation of the crystal across the volume. So, as a result you have so if you if you if you now divide this into several regions.

Let us say these are the regions. Here it is like this and here it could be some other orientation. If I take only the closed pack direction, the closed pack direction in this case is this. This happens to be here; in this case it is happens to be here; in this case it happens to be here; in this case it happens to be here.

So, it is all over the place right. So, the same h k l direction has different orientation in different places and these regions which depict different regions of different crystal orientation they are called as so, these are called as grain boundaries and these are called as grains. So, one region of uniform orientation is called as a grain and where the orientation changes abruptly between the two regions they are called as grain boundaries.

So this is a grain, this is the grain, this is the grain, this is the grain and these are the region the boundaries between them are the that discontinuities are the abruptness between the two is called as the grain boundary. So, this is called as a poly crystal ok; poly crystal and in or you can say polycrystalline material most materials happen to be poly crystalline ok. So, grain boundaries do exist in most materials.

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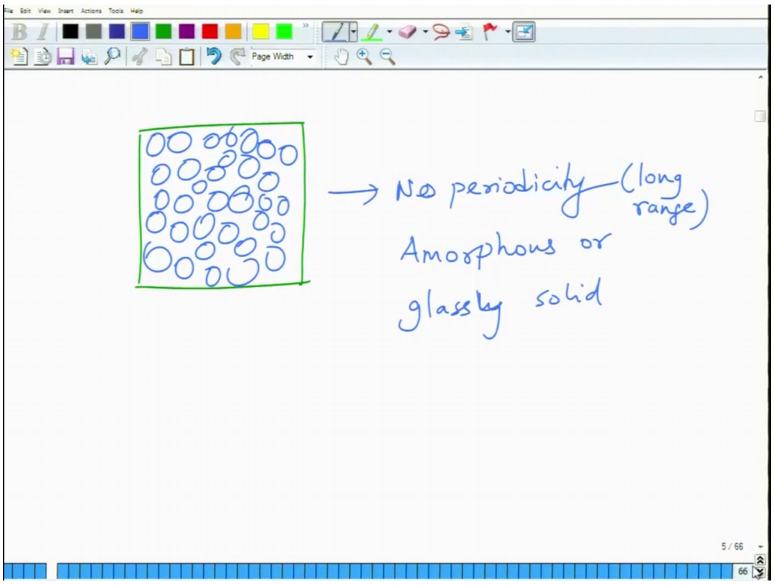

And in some cases you can have atomic structure which is there is no periodicity ok, no periodicity at least no long range periodicity and as a result this is called as amorphous or glassy solid ok. So, these are the three classes of materials which is basically dependent upon the length scales over which the atoms are arranged in certain fashion.

So, in a single crystal and the atoms are arranged in a uniform orientation across long length scales that is what makes single crystal. It has a uniform orientation all across the surfaces on every face of the specific orientation, a specific arrangement of atoms.

In a poly crystal, the arrangement continues only within a grain which could whose. So, the dimension of grains can vary between few nanometer to typically few microns. It could all be few millimeters, but generally it is limited to microns ok; few nanometers to few microns. This is a polycrystalline material. The moment it goes to millimeters it we call it a quasi single crystal because you can break the material into small small single crystals ok.

So, that is why we say it is few nanometers to a few hundreds of microns. And then we have absolutely no periodicity or no long range periodicity. There could be periodicity on short scales like 5 nanometer or so, but the moment you cross that barrier it is there is no periodicity; these are amorphous structures. So, you can see that for example, in this structure there is a discontinuity at these regions; these regions are defects which are called as grain boundaries. But there are a lot of other kinds of defects which are present in the materials as we will see in the next few slides.

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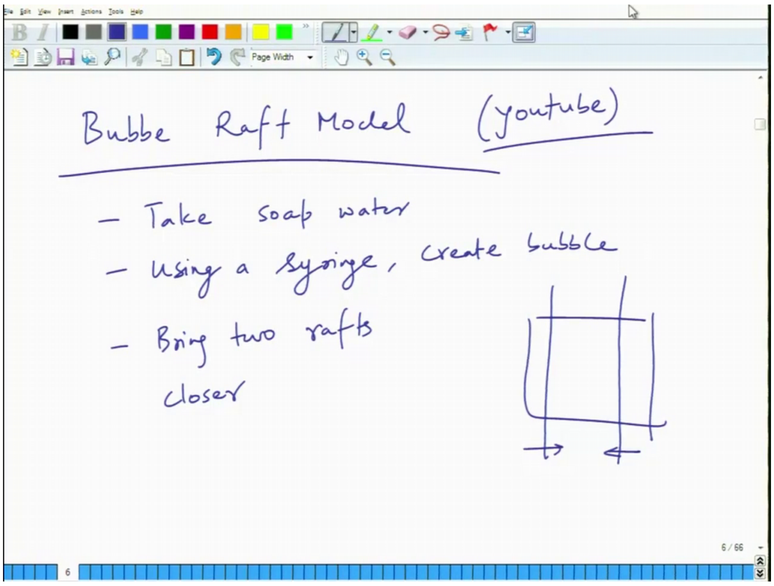

So, the one of the best representation of defects can be seen in what we call as bubble raft model. So, what you do is that basically you take the soap water. So, I will just write this step ok; take soap water, using a syringe create bubbles, just like just blow air into the soapy water and then bring two rafts. So, rafts are located like this.

This is your liquid, these are your rafts bring the rafts closer to each other. So, that all the bubbles are within a region. So, so bring that to bring two rafts closer and then you will see the soap because each bubble can be considered as an atom and then you see the arrangement of these bubbles within a periodic space how does it look like.

It looks like pretty much like atoms arranged in a lattice, but it will show you the kind of defect for example, it produces I will show you slide where you can visualize this.

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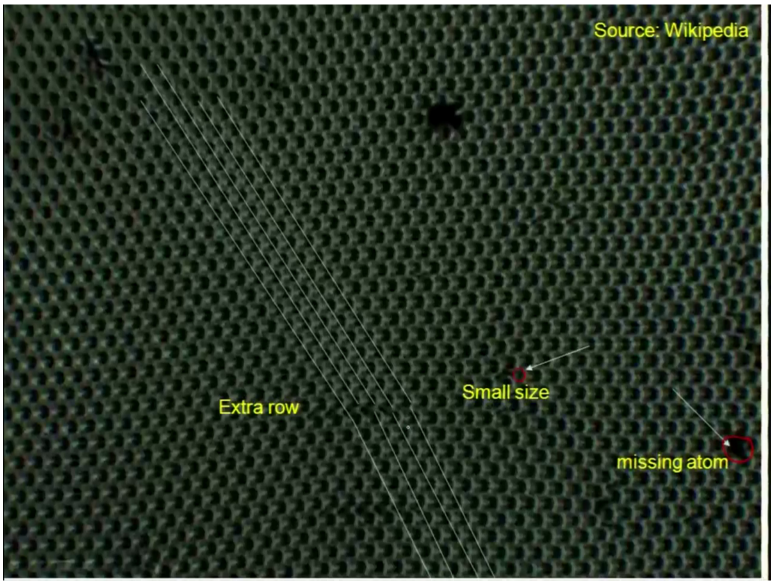

So, this is for instance a bubble raft kind of thing. So, this is the bubble structure which you have created by bringing the bubbles together. So, you can see that astonishingly they look like as if you know you have a bunch of atoms, but these atoms when they come close to each other they are not perfect; the arrangement of these atoms is not perfect.

For example, you can see a small bubble sitting here. It is like a small impurity right interstitial atom; you have a missing atom here on the right side ok; so, this one on the right side. Now, let me use a pen. So, this is the missing bubble which is like a missing atom. You have this is small thing here which is like a small size interstitial atom and when you join these rows together you see that here you have 5 rows of atoms and here you have 4 rows of atom.

So, there is sort of a extra row which has been squashed in between and likewise if you do a close analysis, you can see lot of defects in this bubble raft model.

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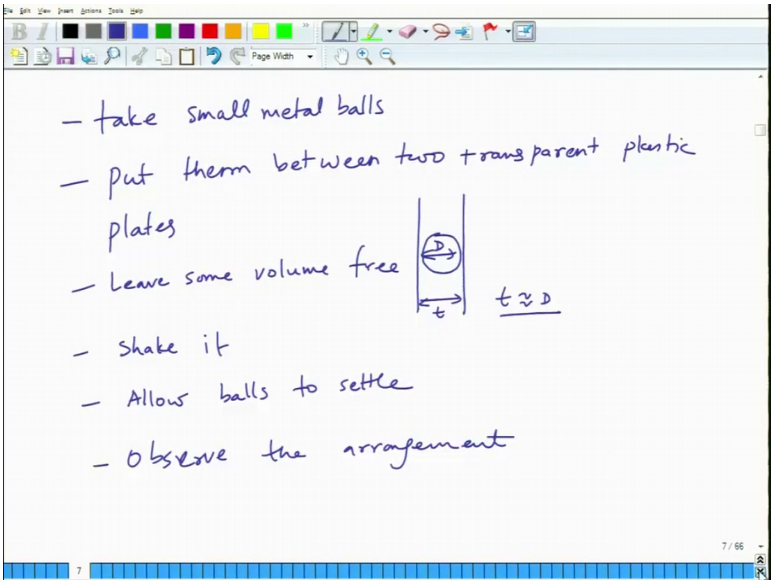

Another way to do it is to visualize this is to take small metal balls ok, hundreds of them and put them between two plastic plates and the spacing between the plastic plates would be same as the metal ball. And just and so, you create enclosure. So, that it is full of metal balls and then shake; it just leave a slight empty space for balls to move around and then you shake it and then let them settle down on top of each other and you will see all sorts of defects forming in the, so, put them between two transparent plastic plates.

So, this is one plate; this is another plate and the spacing between the plates is same as the diameter of the ball ok. So, this is the thickness spacing; the t is nearly equal to D. Leave some volume free so, that balls can move around. Shake it and then allow balls to settle and then observe the arrangement because each ball can be considered as a atom.

You will see a similar kind of pattern as I showed you in the previous slide in the slide here. So, what you see here will be very much replicated in this. So, this is an experiment you can do at home. Bubble raft model you can also look at you can go to YouTube and there are a lot of experiments which have been done using bubble raft model that you can look at. So, if you do this exercise what we will see is that there are a few kinds of defects that we observe.

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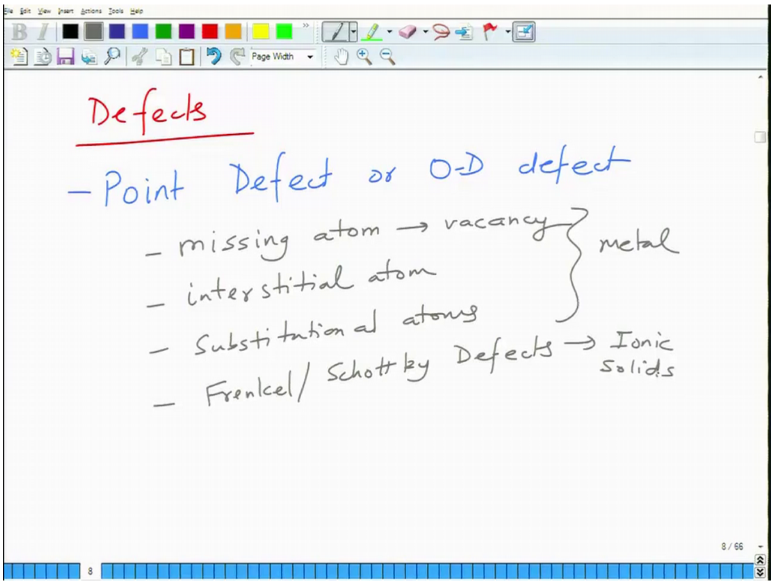

The defects that we observe are categorized in three categories. First kind of defect that we observe is called as point defect or zero dimensional defect. Basically, what we see there is a missing atom which is called as a vacancy. So, we are mostly going to talk in terms of metals, but the same could be true about the ceramics as well, but making sure ceramic is electrically neutral ok.

So, you have a missing atom and then you can have an interstitial atom and you can have a substitutional atom. This would be true in case of metals and other materials. In case of ceramics you can also have you can have defects such as Frenkel defects and Schottky defects; ionic solids ok.

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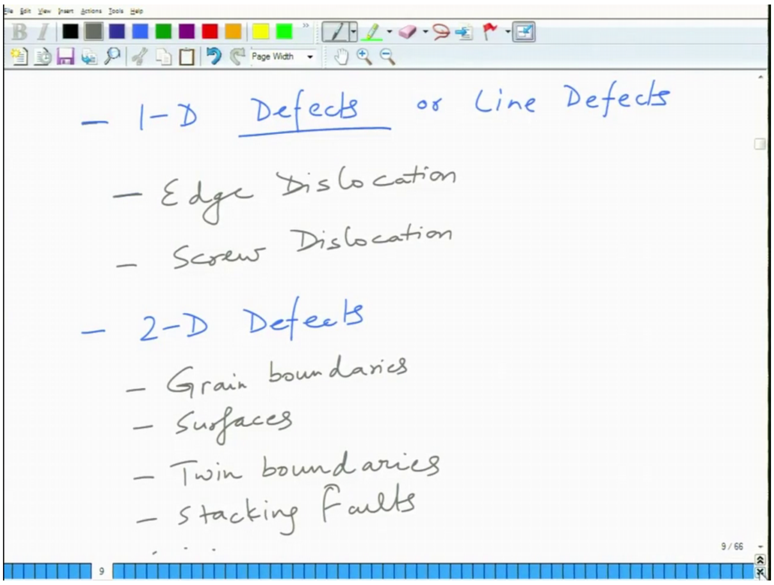

The second level of defects in terms of dimensions would be 1-D defects and here we talk about line. So, these are also called as line defects line defects. So, here the categories are edge dislocation and screw dislocation and third category of defects is called as 2-D defects or which are called as surface defects and here we talk of defects such as grain boundaries. In general surfaces, surfaces are because they have dangling bonds that is why they are also defects.

In general surfaces you can have twin boundaries, you can have stacking faults, etcetera. There are many other 2-D kind of defects. Perhaps would not be able to discuss all of them, but we will see some of them ok.

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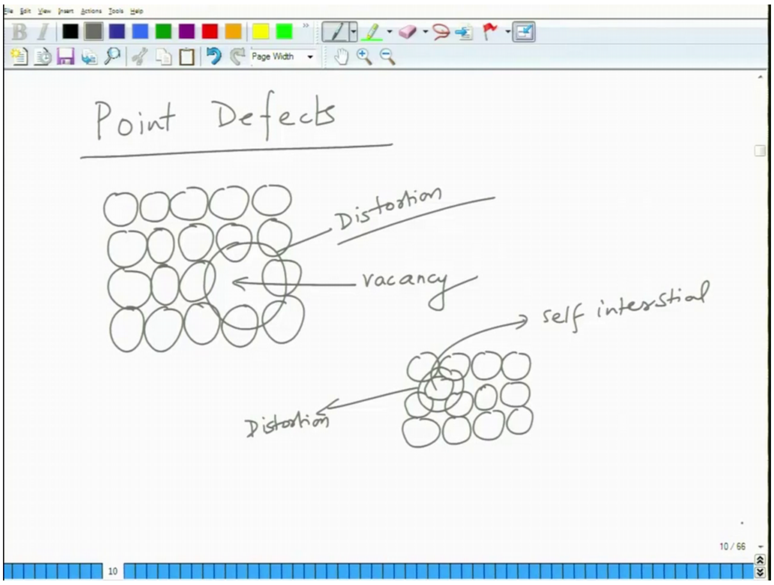

So, now let us first begin with the point defects ok. So, in this category of defects we first consider the vacancies. So, vacancy basically it would be you have you have a structure of atoms like this. They make a periodic structure and if one of them goes out, let us say this guy goes out. So, this is a vacancy ok. You can have a self interstitial for instance you can have a structure again in this fashion.

There is one atom which is squashed somewhere here of the same type; it is squashed somewhere here, as a result it has dilated the lattice to some extent. So, there is a lattice distortion this is called as self interstitial. So, as you can see if you have a vacancy you will have some distortion in the vicinity of the lattice. This will lead to distortion. It will have a strain field similarly if you have this atom it will lead to distortion right.

So, in one case you will have compressive stresses, in other case you will have tensile stresses. Here you will expand the lattice; as a result the resulting stresses will be compressive stresses. Here you will compress the lattice; as a result resulting stresses would be tensile stresses. So, they will lead to their own stress fields. So, these are two kinds of defects. Another kind of defects could be substitutional atoms.

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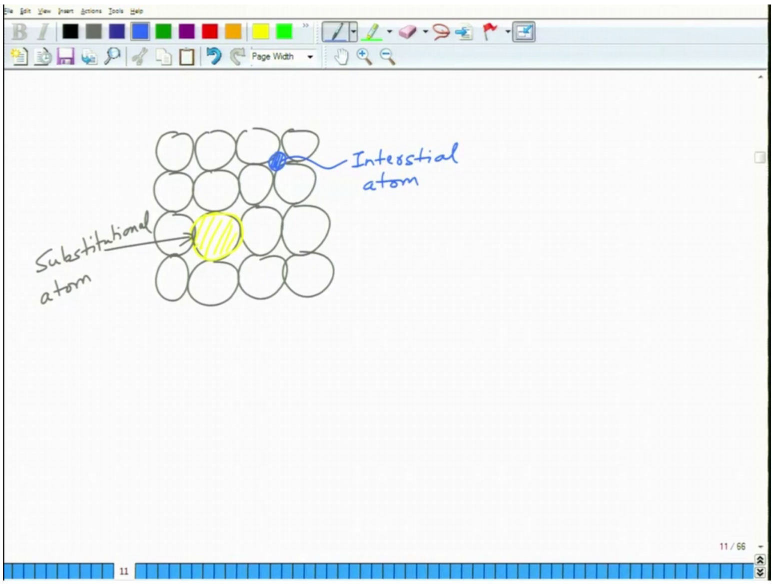

So; this is your normal structure of a metal or material and let us say I replaced one by a different one. So, this is my this would be substitutional atom. It is also a point defect; depending upon the size of this atom that can create tensile or compressive stresses. You can have a interstitial atom sitting here. Again it would give rise to stresses depending upon the size of this atom with respect to the void size ok.

So, these are various defects that you may have. These defects may exist together. They may they may exist independently depending upon the type of impurities that you have present in the material. In case of ionic solids what might happen is that, in case of so, these are the defects which are present in all sorts of materials.

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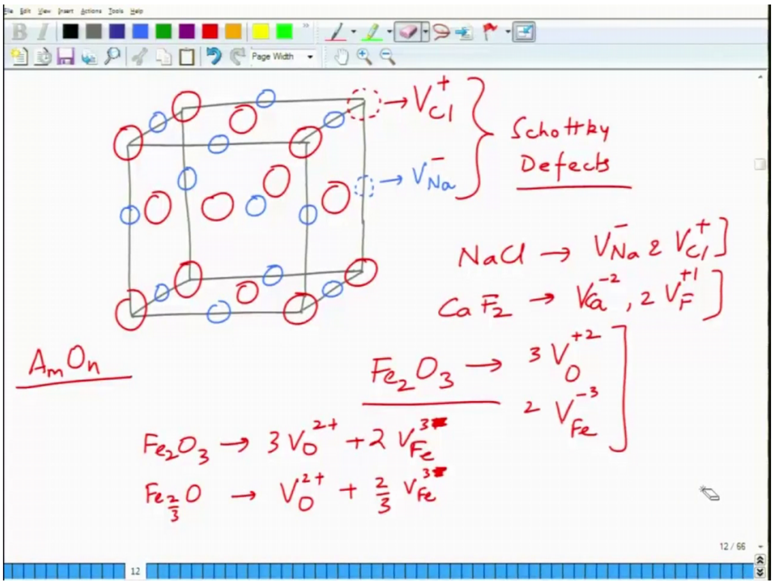

As far as ionic solids are concerned let us say you have a ionic solid. So, the first ionic solid is the best in ionic solid that we know is NaCl ok. So, in NaCl we know that chlorine goes to face centered sides and sodium goes to interstitial sites which are these ok. Now, here what might happen is that if you if you if you if you if you move if you remove one, one of these atom; then to maintain the electrical neutrality this also goes away.

So, as a result what you will have is you will have you will have this as a vacants. So, this is this is V Cl and what you will have here is Na and these are charged; V chlorine is charged oppositely as of chlorine ion. So, this will be positively charged, this will be negatively charged and this is called as the pair of these is called as Schottky defects.

So, in case of sodium chloride it would be V Na and V Cl. In case of calcium fluorite it would be V Ca minus 2 and 2 V F plus 1. If you have Fe 2 O 3, it would be, so, you can have basically and so, you have 3 of oxygen vacancies which will give you plus 2 and 2 of iron vacancies which will be minus 3. Maintain the charge neutrality; the charge neutrality is to be maintained. So, you have Fe 2 O 3; which is analogous to saying you have 3 V o 2 plus plus 2 V Fe 3 plus or you can say it is.

Student: Minus 2.

You can say Fe 2 by 3 O ok. So, this becomes V o

Student: 2 plus 3.

2 plus plus.

Student: 2.

2 by 3.

Student: 2 by 3.

V Fe 3 plus.

Student: 3 minus.

3 minus sorry; this will be minus here. Accordingly you can have the so, the for a for a for a solid A m O n you can have accordingly the formulas written alright. So similarly you can write for AO2 and things like that. So, this is the way you write the Schottky defect; then you can have Frenkel defects.

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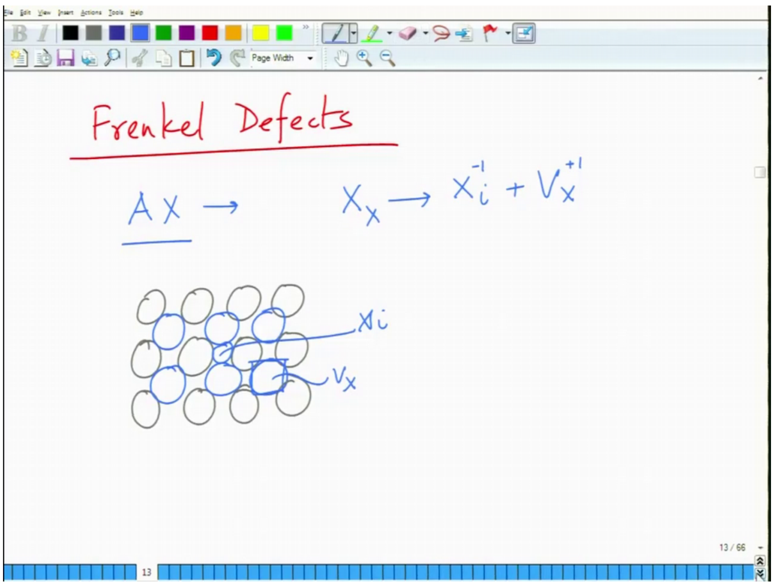

Frenkel defects are other kind of defects in which you have so, if you have a solid AX then the X from X site goes to X interstitial creating a.

Student: Vacancy of X.

Vacancy of X. Since X is a cation ok. So, in this case Xi would be negatively charged. So, let us say if it is charge 1 then it would be minus 1 and this would be.

Student: Plus 1. .

Plus 1; So, your structure so, if you can have my structure like this; let us say ok. Your interstitial ion is this is your X ok. This X has gone missing from it is own site. So, this is now you can say vacant, this is VX; it has gone somewhere here let us say this is your Xi ok. So, this is your interstitial, this is vacancy.

Student: Yes sir.

This is our called a Frenkel defects and there is another category called as anti Frenkel defects; where a cation and it happens with that if that is the same happens with the cations ok. So, these are the so, you can have basically what you can have is cation interstitial, cation vacancy, anion interstitial and then vacancy.

So, variety of defects are possible. In case of in case of ionic solids, it is important that you maintain that charge neutrality.

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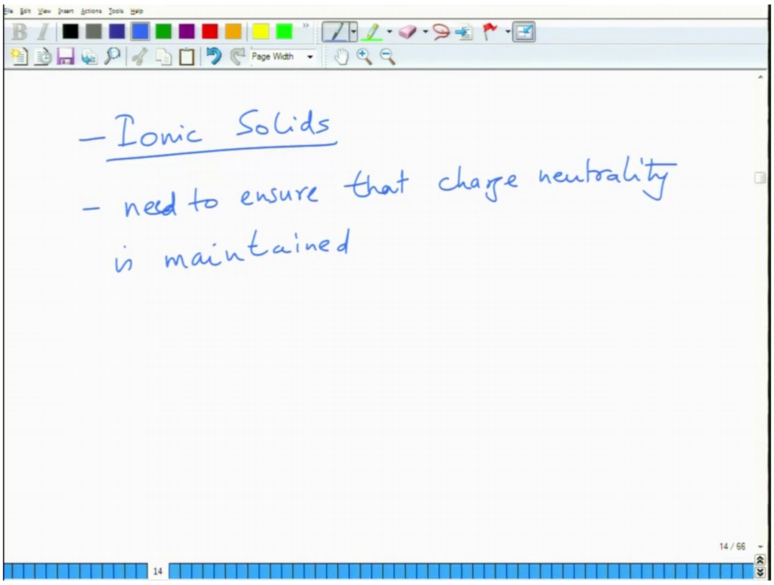

So, in case of ionic solids let me just write it here; ionic solids need to ensure the that charge neutrality is maintained and mass is conserved ok. So, this is about the point defects. What we will do next is some discussion on some discussion on the concentration of point defects in a material because and we will also see that these defects are equilibrium defects which whose concentration is determined by the temperature.

So, at a finite temperature every material will have point defect no matter what the situation is. So, these are all so, point defects as we will see later on their thermodynamic defects. You cannot eliminate them, you can reduce their concentration by changing the temperature, but they do exist ok.

So, what we will do is that we will do a simple thermodynamic analysis in the next lecture and calculate their concentration in the materials ok.