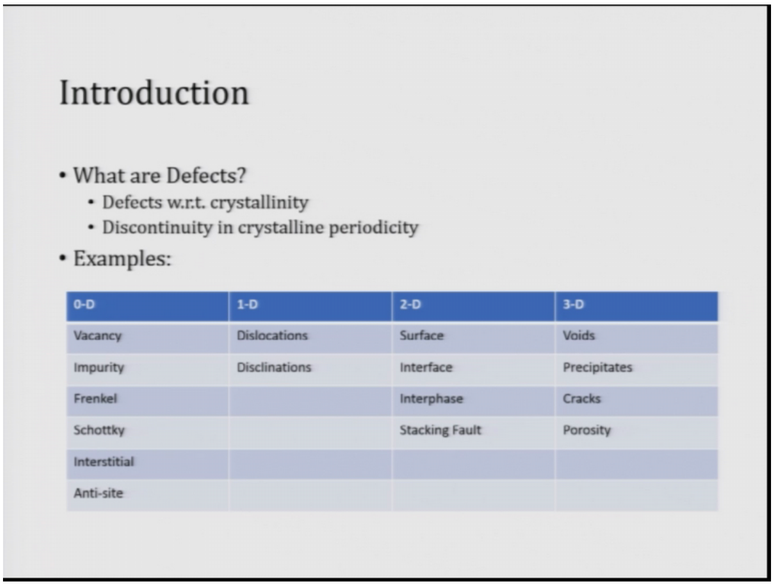
Defects in Crystalline Solids (Part-I)

Prof. Shashank Shekhar
Department of Materials Science and Engineering
Indian Institute of Technology, Kanpur

Lecture - 01
Introduction to Defects

Hello and welcome friends, I am glad that you have joined this course on Defects in Crystalline Solids. So, as it says part I because this is a little extensive course. So, it has been divided into 2; 20 lecture courses and this is first part of it. I am hoping that you have gone through the intro lecture that was the intro video that is posted on the course website. I am Professor Shashank Shekhar, I am Professor in Material Science Engineering at IIT, Kanpur ok. So, let us get going with the brief introduction to this particular course.

(Refer Slide Time: 00:57)



Let us start with what are defects? W e are talking about defects in crystalline materials ok. So, defects can be of many kind; it can be related to non-structures also, it can be related to topography, it can be related to many other aspects defects in many other aspects, but when we are talking about defects in this particular course; we are talking about defects with respect to crystallinity.

Now, what do we mean by defects in crystallinity? Defects in crystallinity or crystalline system is whenever you get a discontinuity in crystalline periodicity. So, it this discontinuity can be of various kinds as you will see; it can be that just one atom is missing or a row of item is missing or maybe that there are all the atoms present, but one of the atoms is of bigger size; that is also a discontinuity now, because the atoms around with around it will have to adjust. So, these are all different kinds of defects and they all of them will have influence on the properties.

So, what are the examples? So, let us look at some examples that we encounter with respect to defects. Here are very wide variety of list and this has been classified based on dimensions ok. So because, we are talking about crystalline; so crystalline material, so it is a very good classification with respect to dimensions when we talk about 0 dimension; it is something related with the atoms or one point lattice defect. So, examples for 0 dimensions would be vacancy when you have a missing atom, impurity when you have a atom present which is not supposed to be there. So let us say for example, if you add in copper there is some antimony present then that will be a impurity.

Frenkel defect; Frenkel defect is when lattice ion moves to interstitial. Now, to maintain charge neutrality; it will always happen that these will always have take place in pairs. So, there will be an ionic as well as cationic ions moving into lattice sites; interstitial sites. So, that is also Frenkel defect and like I said since we are talking about an ionic and cationic, it means that usually Frenkel defects are associated with ceramics or anionic or charged ionics a kind of systems.

However, you can also define it in a metal. So, whenever atom moves from its original site to a interstitial that can also be defined as Frenkel, but that is a very mundane definition of Frenkel. The real or the more technical or the more accepted Frenkel is when you have ions moving into interstitials; then we have Schottky vacancies of opposite sides. Now, here both the cations and anions and again like I said this is we are talking about cations and anions here means which means we are talking about ionics materials. So, when both cations and anions are missing from the site meaning vacancy for a cations, vacancy for anion is present as a pair then it is called Schottky.

It need not be exactly at the same place, it may it is just that for maintaining charge neutrality you would know; you would know that on an on a whole the vacancy fraction of anions should be equal to vacancy fraction of cations; at least in terms of charge. So, the total charge carried by vacancy anions would be equal to total charge of vacancy cations. Interstitial; now this can be defined for a pure material also, when a atom moves away from its site and into interstitial that will be interstitial defect. Now, this can happen because either the material itself has gone into the interstitial site or another ion or another atom which is are forming an alloy with this is going into the interstitial site.

In many a cases this kind of defects can exist as a homogeneous alloy. For example, iron carbon alloy iron in the, in this iron carbon alloy carbon is always at the interstitial site. So, this defect is actually present homogeneously in the system and giving it the overall properties; different from iron and we get a steel iron carbon is steel. So, this alloy is forming because of this kind of defect. Still another kind of defect 0 D defect is anti site. For example, in gallium arsenide, gallium may be sitting at arsenide; arsenide place and arsenide sorry the arsenide may be sitting at the gallium site. So, this is the and wrong atom at the wrong place both and again this has to occur in pairs. So, this is the anti site 0 D defect, meaning only at point defect 0 D is point defects.

Now, let us go to another dimension which is 1 D. So, here row of atoms or row of defect would be found and the most common or the most encountered example in this category is dislocations. Now, in this dislocation itself as you would later see in the course are of two types; screw dislocations and edge dislocations. In both of them there is a line of atom which is missing or the structure around it gets changed.

So, this is a different kind of defect; related to dislocation, but very different from dislocation is disclination. You can think of it as a twist in the crystal; so, the stress will occur around one axis and that axis defines the line of defect in disclination; so, again this is a 1 D defect. And it is very different from dislocation; with dislocation usually have a small range effect while disclinations have a long range effects.

Now, let us move to one dimension higher and then we get to 2 D; surface now I said discontinuity in crystalline periodicity is a defect. So, as you can realise that you are moving in from the bulk when you reach the surface; suddenly the atoms have moved away, there is no more atoms over there; so, this is discontinuity. So, in that sense surface is also a defect and it is not only in that sense because even otherwise you would see that the characteristics that you find for a defect like energy, forces all these also exist with surface.

You have surface energy associated with it; then because of the presence of this defect there is a relaxation near the atoms because on one side there are no more push and pull of the atoms, on the other side there is push and pull of the atom. So, on one side where the atoms are there they relax. So, that leads to the defect which we will call as surface defects.

Interfaces; now even in site material single let us say we are talking about a single element material, let us say copper. Even in a copper the crystallinity does not extend all the way from one end to another end ok; the there is a break in periodicity. And these regions of uniform periodicity are called grains and they are interrupted by grain boundaries or interfaces. So, there are; this kind of boundaries which are called homo phase boundaries, meaning the 2 phases which are being separated with by this boundary by this interface, by this plane are same; so, it is a homophase interface or homophase boundaries.

The other kind can be interface for example, let us talk about duplex steel; now here you have 2 phases austenite phase as well as the ferrite phase. So, one is BCC sorry austenite is FCC and ferrite is BCC; now you whenever there is a boundary between these two, the crystalline structures are different on both the sides. And this kind of boundary which differentiates or which interrupts the continuity is called hetero phase boundaries or interface boundaries.

Still another kind of 2 D defect in materials is the stacking fault. Now, this stacking fault we will get to know more when we talk about dislocations and past particularly the partial dislocations. It is more to do with there is a particular layer by layer arrangement for example, abc, abc arrangement that you see in fcc or ab ab arrangement in fcp. However, if this stacking is interrupted then or for example, instead of going abc, it goes aba then there is a change in the stacking layer.

And because of this there neighbour nearest neighbour or the next nearest neighbour gets changed and lead this leads to increase in energy and this itself is a defect. So, this stacking fault is also related to partial defects or the partial dislocations in FCC materials. Let us get to the 3 D defects; 3 D defects are voids for example, what does what are voids? When you have culmination of several you can say vacancies or in fact, missing atoms from one place then they form void. But these voids are not found just like that; sometimes they can be formed because of cluster of vacancies, but they are also formed because of let say plastic deformation; there can be voids getting formed another 3 D it defect is precipitates.

So, for example, if you have a material which forms precipitate at certain temperature or certain condition; then this new phase appears as precipitates. And this appearance of a different phase which will have different crystallinity, different properties this will lead to a change in the continuity of the matrix structure. So, again this is a defect and this will again in fact, in most cases as we will discuss later particularly aluminium system precipitates are very useful because, they impart additional strength through material.

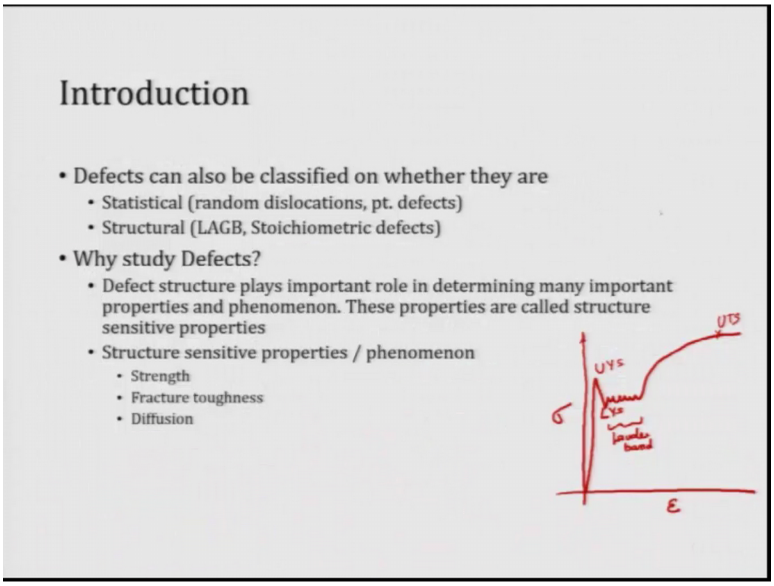
Cracks are another defect; so, this is for example, if you have let say instead of precipitates; you have inclusions which have very large in size and which generate large amount of stress in the matrix, then these large amount of stresses can open up or lead to opening of cracks in the material. So, these cracks are also defect which are 3 dimensional in nature; it will have a very very large scale, it is not in the same it is not of the same order as atom or site it is much larger in that sense and therefore, it is a 3 D defect.

Porosity; so, for example, people who work in portal metallurgy they would know that when you are trying to centre materials; not each and every region gets filled up. And those regions which do not get filled up are called porosity; so this is again something like void, but its origin is different and it is; it has a you can say very different properties; so, leading to different properties and therefore, they are categorised separately like porosity.

So, this is not exhaustive list; in fact, the list of defect that I have mentioned here they themselves will have several sub topics under them. And we will not be able to go through all of them, but what we will do is; we will be going through some of the important characteristics. And as you would realise that when we are talking about material properties, particularly the mechanical properties dislocations are the ones which make the most important difference to properties and therefore, a lot of time would be spent on dislocation.

We will also be spending time on vacancies and other that kind of defects; however, like I said that a lot of time would be devoted to dislocations. And material properties like mechanical behaviour that are influenced by these dislocations and this can be this will be extended to certain extent to 2 D and 3 D defects.

(Refer Slide Time: 13:31)



In the previous slide, we classify defects on the base on the basis of dimensions, but they can also be can be classified on whether they are statistical; something like random they have to be there just because of for example, point defects they are thermodynamically stable, structure. So, they will be present at a particular temperature in certain quantity; so they will be statistical defects

So, random dislocations; will also be counted in statistical defects, they are homogeneously distributed, point defects are another ones. Another category in this is whether they are structural defects means they are whether they are presence causes certain particular kind of structural change in the material. So, they are not really homogeneous in that sense.

For example LAGB or Low Angle Grain Boundaries; when they are present they are they lead to some geometrical deformation or geometrical change in the orientation. If you have a random dislocations; they will not cause any particular orientation change, but when you have low angle grain boundaries which is a array of dislocation; arranged around a certain order or a certain kind. For example, one over the other then it leads to change in the miss orientation between the neighbouring parts and therefore, they are called structural defects.

Now, let us get to the topic of why do we need to study defects? Obviously, we have said that it influences properties. So, defect structure plays important role in determining many important properties and phenomena. And the properties and phenomena which are influenced or which are which are sensitive to defects are called structure sensitive properties and phenomena.

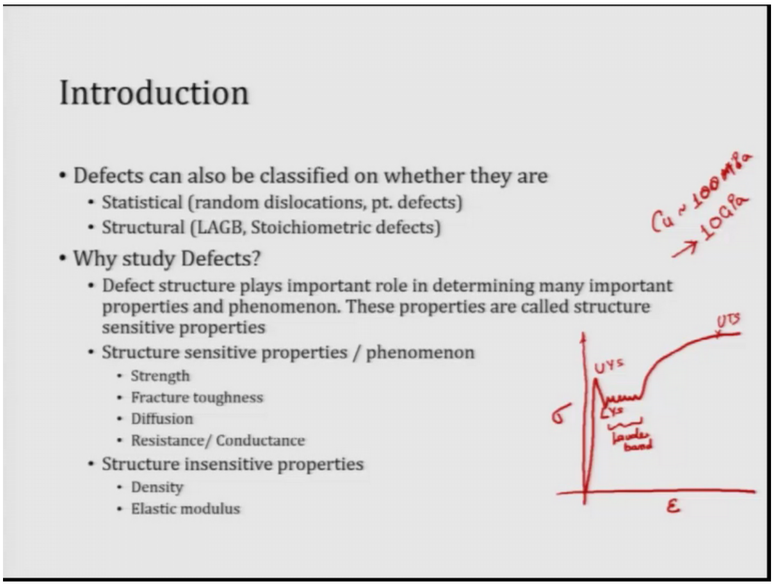
So, with what are those structure sensitive properties? Like I said some of the mechanical properties are the most sensitive to structure; for example, strength yield strength and if you remember in mild steel what is the kind of yield strength or the tensile plot that we get if you remember it is. Let me draw it over here; so, this is a stress train curve for mild steel and why is it like this? We will understand it in more detail later on, but for now let me just tell you that this is because of interaction between point defects and dislocation.

So, the dislocations get fixed up end because of the presence of pen because of the presence of point defects and because of that you need a much larger strength which is called upper yield strength. Now, once these dislocation starts to move then it come then the yield strength of the material drops and we get to lower yield strength. And this band which is nothing, but extension which is that how much region is getting this mobile dislocation is called laude band.

And beyond this once all of the material has uniform dislocation; mobile dislocation then the material start to be have in a common way, just like you would expect for any other let say aluminium system; how they are yield strength or stress train curve would vary. As you keep increasing the strain, there will be work hardening and then you will reach a UTS and so on.

So, this is a very good example of how properties get influenced by defects. In fact, even more fundamental to this is that if you had no dislocation present in a material do you know how much would be its strength? For example, copper yield strength is of the order of 100 Mega Pascal.

(Refer Slide Time: 18:18)



However, if you were to have a copper material without any defect do you know how much can you expect how much is strength should be? It would be of the order of 10 Giga Pascal. So, that is the kind of difference defects make; so sometimes defect can be useful for you, sometimes defects can be bad for you. So, just imagine a world where we had materials without any dislocations and we would have very very high strength material.

But unfortunately or unfortunately there are dislocations and because of which the actual strength of these copper materials are so smaller. Fracture toughness is another of those properties which are influenced because of the presence of defects. For example, if there are lots of voids then the fracture toughness would be much smaller. And you can do photography to characterise, to understand how many defects were there, what kind of fracture you obtained because of the presence of these defects also inclusions can reduce like I said inclusions will lead to crack growth; so, that can also reduce fracture toughness. So, all these defects do influence the properties.

Now, let us talk about some phenomenal diffusion if you have a 2 D structure, 2 D defect like interface or a 1 D defect like dislocation line; the diffusion is known to be much much faster along this region. And why is it? Because the overall volume available around this; defects are much much larger. And therefore, the atoms find it much easier to migrate or hop around these places; therefore, diffusion becomes much faster.

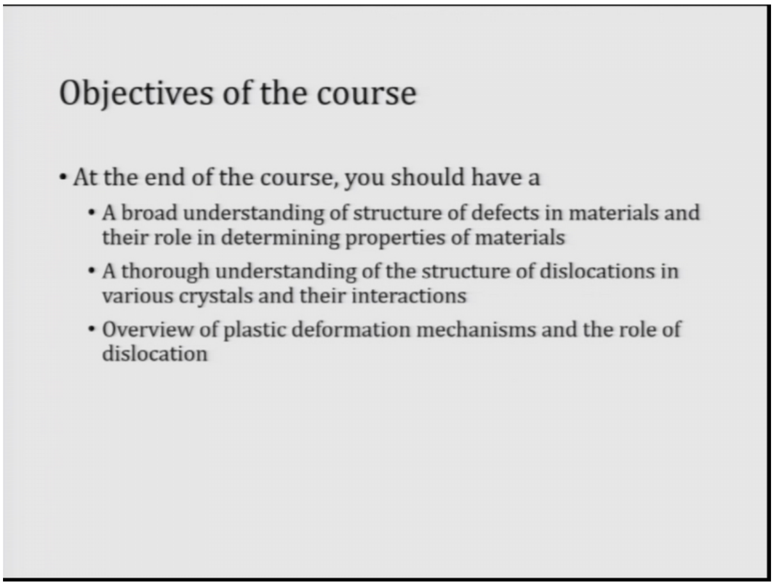
And in fact, we have diffusivity coefficient for dislocation or diffusivity related to; dislocations, diffusivity related to grain boundaries; diffusivity related to triple junctions because defects are getting; they are all increasing order of defects where there have you can say increasing amount of volume for atoms to jump. And therefore, the overall diffusion rate becomes faster; these are mostly mechanical and functional properties, but we also have electrical properties like a resistance.

If you have a lot of defects in a material then their resistance increases or in other words its conductance decreases. Because a lot of the most of these conductivity is taking place because of movement of ions or electrons; in if it is material as if it in the ionic material then by ions and if it is other material then by electrons. Now, if they if you have lot of defects then a lot of scattering takes place of these electrons and because of this the resistance increases. And if we are talking about ionic materials then their movement gets impeded or mobility decreases and therefore, again resistance increases or conductance decreases. But there are also certain properties which to you can say a large extent are insensitive to structure; meaning defects will not be able to influence this.

One and one of the most important one is density. So, you may have point defects and you may think that why should have density not decrease. However, the defects that we are talking about are a very very small fraction of the total lattice sites present. In for all practical purposes we will never be able to reach a region or a range, where you will have significant fraction of point defects or for in that matter any of these line defect, which can increase the overall volume and therefore, density can be termed as structure insensitive property.

Similarly, elastic modulus it is directly related to the bond strength and again the fraction of impurity or the fraction of defect that we have added is so small that you should not; you would not in see any real change in elastic modulus. So, these 2 properties these are 2 examples of properties that is that can be termed as structure in sensitive properties. So, now that we have I have introduced you to the basics of defects; let me bring you to what is the objective of this course the, what are the objectives of this course.

(Refer Slide Time: 23:19)

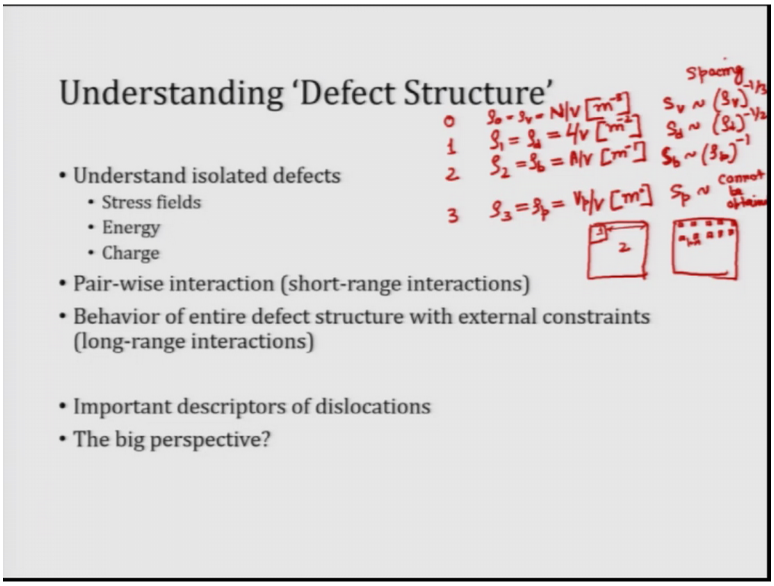


We hope that at the end of this course; you should have a broad understanding of structures of defect, how the defect structure looks like; whether it is we are talking about point defects, line defect play; interfaces or to voids or any of the 3 D defects and their role in determining properties of materials. A thorough understanding of the structure of dislocations in various crystals and their interaction so, as you will see that when we are talking about this course, we have already said that as large emphasis will be on dislocation because our most of the mechanical properties are influenced by that.

So, you must also at the end of this course be able to understand the structure of dislocation in more detail in a much greater detail in various crystals and their interaction and, minima and also their individual properties not just the interaction, but also there individual properties. And since we are talking about dislocations; so, also the overview of how this is the dislocation influence the overall plastic properties of the material plastic; when we are doing plastic deformation, then how do these defects play a role in that.

Now, by the time that you are watching these videos most likely most all these lectures have been recorded, but I would insist or I will argue that whenever you feel that there are certain aspects that you need clarification on; do feel free to contact and we can always add some tutorial modules at a any stage to be able to help you on this.

(Refer Slide Time: 25:02)



Now, when we say understanding defects structure what should be the way to go ahead? How do we proceed for this? First what we need to do is understand isolated defects. So, whether we are talking about vacancies; so, how does the vacancy behave when it is present in isolation; meaning the whole crystal system there is one only one vacancy. So, first we read to understand isolated defects, understand there stress fields, understand how what is their energy, what is the formation and if there it is a charged unit then what are the charges present on it. Then we get to the next stage; now we have understood the structures of one unit how do they interact with in pair.

So, let us say we are talking about dislocation; dislocation or vacancy to vacancy how do they interact in pair or maybe how do the point defects or the vacancy interact with the grain boundary. So, these can be termed as short range interactions meaning that even if you take a real material; then there will be lots and lots of these defects present of different kinds. And when we are talking about pair-wise we are saying how do they at a very small scale what is the influence of these interactions? For example, what is the influence of this point defect and the dislocation. So, this will give you short range properties or short of interaction behaviour.

Then this understanding would be extended to understanding behaviour of the entire defect structure with external constraints. So, now we have the whole system; there are let say there are so many other dislocations present or other point defects presence in that entire system what is the behaviour of this dislocation? For example, dislocation dynamics how do the dislocation move and there are so many other dislocations present in the region. So, that is the you can say path to understanding defect structure; this is the modus operandi that we will follow to understand individual defect; individual defects.

Important descriptors of dislocation now here let me introduce you to some of the important some we have talked about different dimensional dislocations. So, let me introduce you to different kinds of important descriptors of these different dimensions of dislocation. So, let say we are talking about 0 dimension dislocation; so, let me say this is 0 dimension. So, what is the density of this? You can say rho 0 or rho vacancy; these are usually given in what units? Number per unit volume; so, these are this is just to understand what will be the usual description or the method description of this defects. So, the units will be per meter cube and on an average; so, let say this is spacing.

So, what will be the average spacing between this? So, this can be; this can be obtained approximate value we can see we are we will never be able to say the exact value because this will be based on other information that you would need. But on an average you can say that if this is rho v is the density then what will be the average spacing and average spacing will can be termed as rho v to the power minus 1 by 3. So, you take a cube root of the density and that sorry in the inverse of the cube root of the density of the vacancies and that will give you the average spacing.

Similarly, you can do it for 1 dimension; so, in 1 dimension let say we have rho 1 which is equal to we are talking about dislocations; I will term it as rho d and the unit here would be it should be length per unit volume. Because it is 1 dimension; so, this will have unit of meter minus 2. And here the average spacing can be given as rho d to the power minus 1 by 2; so inverse of square root of dislocation. Similarly when we go to rho 2 dimension which is like a plane or a boundary; so I will call it rho b; it is now area per unit volume and therefore, unit will be equal to meter minus 1 and here the average spacing would be equal to 1 over this value. So, we will have minus 1 and these are all units of meter because we are talking about spacing.

However when we get to 3 dimension defects like voids then it becomes a little difficult. And for example, let us say void or particle then here we have volume of particle by volume and here the unit itself is 0. Now this is little bit difficult to find spacing because let us say we have 20 percent fraction of an one phase. So, this 20 percent fraction can be distributed in different ways it can be all in one place or it can be distributed like very very small fractions. And hence the average spacing cannot be obtained from just the information of rho p; in any situation, not as a not even as the average value. So, we cannot sorry the not the rho p, but the average spacing. So, the average spacing between these particles cannot be obtained from this information.

So, as you can see that this is one phase, this is second phase and it can be distributed in different ways and depending on that the spacing would be different. So, here this will be the spacing here this will be the spacing; so, here that because of that we will not be able to find the average spacing just based on this information which is the volume fraction which is V p by v ok.

So, this is some important description of dislocation and before end this lecture; just a important aspect the what is the big perspective? One must understand that a complete understanding of the defects is still missing is a; for example, even a point defect how they actually affect the structure around it is a still a topic of debate and it is not really 100 percent understood in all the materials.

Therefore, the you must keep a big perspective in a mind that what we are studying our simple models to be able to predict some properties and phenomena based on this. So, with that introduction we will come to this end and next lecture; we will start with one of the defects.

Thank you.