Defects in Crystalline Solids (Part-II)

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Lecture - 11
Dislocation Structure in Superlattices

Today we will be discussing Dislocations in Super Lattices. So, what are what do we mean when we say super lattices? We mean that whenever you have two or more species present and they are in a ordered structure. When we, so what is ordered structure will see because there can be ordered as well as disordered structure.

So, the first thing is that when we talk about dislocation in super lattices then when there are, when there is ordered structure of two or more species. We will understand in more detail what we mean by ordered, but for now it is just that there is a specific position for each of the species that is what is meant by ordered species, I mean elements.

Now, this why is it different? Because now there are different positions assigned to different atoms so it becomes more complex, but we have already seen a more complex system like ionic system. So, it is not as complex as that, but it is more complex than simple systems like FCC, BCC, etcetera, ok. So, to begin with we will see some example of superlattices. What are some of these super lattice structures? There is a designation or a name given to each of these. One of these is B 1 structure. And how does it look like? This is our something like NaCl or rock salt structure.

So, this is something that we saw in our previous example when we were discussing the ionic systems. So, ionic systems are also ordered structure system. So, you can say they are also super lattices only that they also have charges associated with them. So, the charges also start to play a role, otherwise rock salt structure, I am not going to draw because we have seen it last time, so it is nothing but interpenetrating FCC lattices of Na and Cl.

So, that is B 1 type of structure. And overall if you look at it this will look like a simple cubic, but it is we should not call it simple cubic because there is a designated position for each of the atom. It is not same type of atom at all those positions.

Let us look at another still another system and which we have not yet heard about and this one is B 2. Some of the simple examples for B 2 are cesium chloride, NiAl. And how does it look like? So, this structure looks like this. So, you can see in this type of system there is one is to one ratio between the two species. So, when you make a structure you always keep in mind that the ratio between the two atoms must be maintained as one is to one. So, one of the type of atoms can take these positions and another atom can take body centered position.

So, you can say this is chlorine and you can say this is cesium, but this is interchangeable because if you connect the two connect all the chlorine atoms it will itself form a simple cube and at the body center of it will become the Cs. So, in this kind of structure these two positions are interchangeable. And therefore, in brief you can say this is two interpenetrating simple cubic structure.

Let us look at few more examples the third one that we look at is given the designation DO 3 and one of the systems that you can see in this is Fe 3 Al. Now, this is also not a very simple system to draw it is complicated in the sense that you have to take into account 4 cells to completely get the full picture. So, this is more like this let me. So, as you can see, I have selected this grid like page because it makes it easier to draw such structures. So, again what is the ratio between the two atoms here, it is 3 is to 1, ok. So, you can assume it to be as if there are 4 cells on the top and 4 cells at the bottom this is what this is structure is actually like.

So, now let me take that this is F e. So, this is much larger in number and where are the position that I will put them all the first all the corners, ok. So, these are at all the corners of these cells. So, this is a corner, this is a corner. So, it goes at all these and there is also something that will go in the center of the cells, but before that I have not drawn this. So, let me draw this and so there is also a corner atom in the center of this.

Now, if there are 1, 2, 3, 4 there are 8 different cells and in each of these at the corner we have Fe. So, how many Fe that would be? So, if you look at only the corner atoms, now each even a simple cubic if the atoms are all at the corner then one cube contains one atom therefore, we here we have 8 corners, so their sorry 8 cells, so there are 8 corner atoms.

Now, let us go to the and it is not complete I will come back to that. Now, where are the aluminum atoms? So, the aluminum atoms now you can see that there are 8 cells, out of these the alternate body centereds are taken by the aluminum atom. So, this body center of this cell, body center of this cell, then again the body center of this particular cell and the one diagonally opposite to this one.

So, that is our red ones are aluminum atoms. So, they are in the body center of half of it therefore, there are 8 cells, so there are 4 of it. But then this does not complete the ratio as you can see there must be some more Fe atoms because we need 3 is to 1 and at the same time only half of the body centers cannot be filled, so other half of the body centers are filled by the Fe atoms.

So, there are 4 body centered Fe atoms. So, in effect this system is not Fe 3 Al, but it is Fe 12 Al 4. So, this is the ordered structure again as, so, you can realize that it is not that anywhere we have put Fe and anywhere Al can go there is a specific position and in fact, in this particular one, it is all the more very specific even the body centers are not all of it taken by aluminum some of the body centers and not again not randomly, but specific body centers are taken by Fe. So, this is called a DO 3 type of system.

Now, there is still another system or another way that your Fe 3 Al can be distributed, but not only Fe 3 even some other material like Ni 3 Al, Cu 3 Au and Fe 3 Al all these are examples of L 1 2 structure. Next one that we are discussing is the L 1 2 structure. So, how does it look like? Well, this is not as complicated as the previous one. So, where does Fe go here? Here at the corners we have aluminum. So, again one cell and include all the corners. So, we it means total of one atom. So, this is actually I should have drawn it in the red color keeping in view the previous diagram, but none the less. So, here aluminum is at corners, which is equal to 1 atom.

Where is the Fe atom which is now being shown by red. So, the Fe atom goes at the face centers. Now, there are 6 face centers and each atom counts as half, so 6 into half is equal to 3. So, face centers is 3. So, again you can see we have we end up with Fe 3 Al. So, this is another kind of system. Now, here instead of Fe you could have Ni and you would get what is called as Ni 3 Al system.

Now, so we have seen 4 different system, next thing that I want you to understand is what is that that there is something called as order disorder transition, ok. So, let me give you an example with respect to our B 2 structure. So, in the B 2 structure if you remember now, this is I will have to draw two systems one the ordered one and the other the disordered one. So, if it was Ni Al which is our, so at the corners here we are putting Ni, this is our, this will be called ordered system and in the body center we put aluminum. So, this is this will be called ordered.

And if you increase the temperature then what you may end up with is a system like this. And what does the blue here represent? Blue here represents that this atom is 50 percent Ni and 50 percent Al. And if you were to talk in terms of crystallography then this structure will be B 2 and this will be BCC, ok. So, in what is the difference here? Here you can see there is no designated place for Ni and Al atom it can go anywhere. Only that since the overall stoichiometry is 1 is to 1, so each of these atoms have a probability 50 percent of being nickel, 50 percent of being aluminum.

And therefore, there is no set order that next to this atom you will have you will find another atom, it can be continuous probability wise you can have a continuous set of nickel atoms at one place at least continuous set of aluminum atoms at another place. And like I said this will be called disordered.

To make things clearer and more relevant from engineering or materials point of view super alloys that I promised I will be discussing is even one more system which is again I have already shown it to you in the ordered form now let me show you as a comparison or how the transition form, order, disorder. So, here like I said earlier you will have aluminum atoms at the corner and this time I am assuming Ni 3 Al and nickel atoms at the face centers.

So, this will this is nickel, this is aluminum, and this is a ordered L 1 2 structure. And how will a disordered structure look like, now I hope you are able to relate or understand what will be different. So, this is the structure that is disordered. Now, like I said what does this blue atom represent here? Now, you should be able to say from looking at this it is still Ni 3 Al overall. So, the ratio must be maintained but there is no designated position, which means that now 75 percent of any of these spots would be filled by Ni

and 25 percent of any of these spots will be filled by aluminum. And this will be called disordered and the structure would be called as FCC.

So, here that is the difference. So, and when do these transformation occur? Usually this will occur at higher temperature. At lower temperature most of these systems would show a ordered structure and at higher temperature they will show you show a disordered structure. And why is it so important one that the ordered structure would show a completely different.

So, let me point out show a different dislocation behavior. Why? Mainly because there can be chemical stacking fault. Meaning, here when you are moving the atoms you also have to make sure that the nearest neighbor relation between two species are maintained, meaning if the nearest neighbor between Ni was Al then it should not become Ni and Ni. So, that will also create, it is not an anti-phase the sites are still the same. So, that is even though the sites are same, but still we just because the species have changed there can be repulsion and that may create another kind of you can say stacking fault, but this is called chemical stacking fault.

Now, that we are talking about the ordered and disordered structure. So, this one is called L 1 2 this is called FCC now do you think you can actually differentiate by any means is there any characterization technique which can say, this is not f this is not Ni 3 l order, this is disordered or this is a ordered fc Ni 3 l versus this is a disordered Ni 3 Al. So, yes there is there are indeed techniques. For example, even your XRD, now XRD is dependent on the crystal structure and FCC will have a different XRD pattern compared to L 1 2 because here all these atoms will behave as if they are a combination of Ni and Al,75 percent Ni, 25 percent Al.

On the other hand, here it is Ni is giving a different cubic system and Al is giving a different cubic system. So, they will have a different structure factor to contribute to the overall diffraction pattern and here it will be just like a FCC system. So, in that sense they will give a completely different XRD peak profile. So, characterization technique can indeed differentiate between these two techniques.

Now, let us come to the more relevant system. And I have some pictures to show you, but before that let me point out some of the things.

$$V = Aexp(\frac{-E}{KT})$$

We are currently in the with respect to this lecture we are interested in ordered inter metallics. And why are we interested? Basic basically, I mean student just dislocation be treated as dislocation. Well, the purpose of dislocation has always been that it will be able to predict some of the or it describes or it defines some of the properties.

Now, here we will see one such phenomena, which is of great importance to engineering. So, in that, so for that reason we are interested in ordered inter metallic system. And what are some of these key properties that they show? So, one of the properties is that high strength, higher strength compared to a simple FCC or BCC system and that to at room temperature. And if the system is appropriate in some of these particular intermetallics you can even see that strength increases with temperature.

Now, this is a very very interesting and useful phenomena and that is why we are able to get so many useful high temperature materials because some of these materials their strength increases with temperature. Usually what do you expect? Ok. So, let us look at what would be the usual, if you looked at a shear strength versus temperature. So, the usual plot that you would expect would be that the strength should decrease and that is what you will see for let us say a simple FCC, BCC system or even a disordered which is just like a simple a BCC system a disordered Ni Al; we are not talking about ordered Ni Al.

On the other hand, if we look at Ni 3 Al then it shows what is called as yield anomaly. So, here you see the shear strength is increasing with temperature and this can be as high as 800 to 1000 Kelvin. So, close to 800 degree Celsius you can see increase in strength and only after that it drops, and that is why you are able to make the turbine blades which operate at some, so such a high temperature out of these super alloy systems because they have strength even at these higher temperature. And this behavior is termed as yield anomaly. So, the strength is increasing and then drops.

And why does the strength drop? Well, there is a very simple reason for that you can look at the equation for velocity of dislocations and that I mentioned earlier and it comes out of this form. So, your stress requirements are in this over here, but what this is saying

in general is that at higher temperature lower stresses are required to keep deforming at same rate. So, if your v is constant and this drops, so it means, so if this value increases when your T increases. So, this must also drop. And that is what it is saying that, that stress required to keep the dislocation moving at the same velocity reduces when temperature increases.

So, this is explaining the behavior of simple systems and that is what we experience all the time that strength decreases as the temperature increases, but not for this particular material the super alloys, ok. So, we will come to this in a moment.

So, now, let us start looking at this what is this super alloy system. One of the super alloy system is Ni 3 Al. So, this is a nickel based super alloy and earlier also I have shown you how this structure is, so at the corner and here again and because it is so much important and we want to understand it fully. So, we want to look at it in more detail. So, you this is a ball stick model. So, you can see aluminum atoms are at corner and the phase centers are the nickel atoms. And remember this is a ordered structure.

And if you are looking at the hard sphere model this is how it would look like. So, again this is, this one is aluminum and the phase centers are nickel. This is a ordered structure. So, let me now come to this system. So, now, you know that this is not really FCC system, but what we called as L 1 2 and not FCC structure.

So, having said that so if it is not FCC structure. So, what is the slip system? The slip system as, so here the short first let us look at what will be the shortest lattice vector. So, it seems that the shortest lattice vector is still the same right along the phase diagram. So, it looks like it is still a by 2 110 type will check, ok.

What are the planes? What are the planes on which the slip takes place? The planes on which the slip takes place are so, here there is some similarity with FCC, there are there is one plane which is similar to FCC which is 111. But then again, the similarity ends and there is another slip system which is 100, ok. So, now, we want to establish whether this a by 2 110 can still be a lattice vector for our Ni 3 Al system.

So, the question here that we want to be asking is it a possible translation vector. So, for that let us select one of the planes 111 planes. So, this is a 111 plane and over here if you look at it this is how it will be. So, this is the 111 plane and now if I draw it in with more

atoms this is how it will look like. So, first let us look at only the darker lines and atoms over there.

So, this is your 111 plane and you can see there is aluminum atom, nickel atom, then aluminum atoms, so aluminum, nickel, aluminum; nickel, aluminum and so on. And again, if you look at the other direction there is aluminum, aluminum, aluminum; and as you can see there are more sorry more nickel, nickel, nickel and these this red ones are the aluminum. So, as you can see there are more nickel atoms which is expected because this is Ni 3 Al.

But then this is not the only 111 plane, there is still another 111 plane below it which forms the nearest neighbor for these atoms. So, if you look at it now here the, this is the second layer which is drawn over here. So, the lighter green atoms are also nickel, but in the second layer. So, the lighter atoms here are. So, let me say this is second layer which is below and the darker regions are the first layer top and let me also write down that this is a nickel atom and this is a aluminum atom, ok.

So, let us be very clear about that. We have two layers that I am showing here the 111 layers, so this is a 111 plane. So, 111 layers I am showing on the top there is one layer, these are the green ones are the nickel, red ones are the aluminum and similarly there is another layer below it and the relative position when you look along the 111 direction is like this. And so these are your nickel atoms and these are the aluminum atoms now where is our a by 2 110. So, this is the a by 2 110. So, this means this will be your a by 2 110.

Now, if you shift by this much now if, so if our dislocation line is somewhere along like this and the burger vector is like this. So, the extra half plane let us assume the extra half plane is on the top and extra half plane moves to the right. So, everything here gets shifted by this much amount to the right. Now, what happens? Does everything remain same? Let us look at x atom, x position and y position.

Now, as of now what you will see is that x; what is x? It is aluminum, it is surrounded the nearest neighbors are all green which means it is nickel. Anywhere you see aluminum atom the nearest neighbors are nickel aluminum atoms nearest neighbor are nickel. But now if you shift it from here to here, what will happen? Now, its nearest neighbor has changed two of it is still nickel, but the third one is no more nickel it is aluminum. So,

there is the sites are still the appropriate sites it is not going in the wrong site, but the nearest neighbor has changed.

$$V = Aexp(\frac{-E}{KT})$$

So, this a by 2 and I am trying to squeezing here because my drawing is over here leads to nearest neighbor fault and this is called. So, if we apply a by 2 110 translation nearest neighbors of aluminum changes implies that a by 2 110 is not a lattice translation vector. Implies and that there will be a anti phase boundary that will be formed.

This is when you have the stacking, there is no problem with the stacking there is only problem with wrong type of atoms being present here, the nearest neighbors have changed or the next nearest neighbors have changed here it is the nearest neighbors which have changed. So, anti phase boundary is created and which has energy of the same order as stacking fault which is 10 to 100 milli joules per meter square.

So, we have found out that on the 111 plane a by 2 110 does is not a lattice translation vector. But what about the other let us say we if we go back and from v c this is red atom, this is red atom. So, what if I move from here to all the way here, meaning I apply a 110. So, now, you can see when if I move red to red, green to green nothing is changing.

So, a 110 is certainly, ok. So, in on 111 plane, but we need to confirm. And we need to confirm by looking at another possible plane. What was the other possible plane? 100. So, we will come back to the other plane. We will come back in the next lecture and discuss about the, what happens when there is a other plane.

Thanks.