Defects in Crystalline Solids (Part -II) Prof. Shashank Shekhar Department of Materials Science and Engineering Indian Institute of Technology, Kanpur

Lecture –12 Stacking Fault and Kear-Wilsdorf Lock in Superlattices

So, we saw that in a Super Lattice system and we are talking about Ni3Al which is also called Li 2 structure. So, over there it looks like FCC, but it is not FCC it is Li2 structure. Ni has a separate position, alumina has a separate position and now because of that if we take a system where 1 1 1 plane is the glide plane and a by 2 1 1 0 is the lattice vector then we saw that it leads to what is called as chemical stacking fault. So, the species of opposite kind are together which is not desired and it is also called and it creates what is called as Anti-phase boundary.

So, we have checked that for 1 1 1, but now we need to also check it for the other plane that is possible in an L12 structure which is 1 0 0 plane ok.

So, this will also confirm whether a 110 that we found to be a translation vector on 111 can be used as a full translation vector for 100 plane and if it satisfies both of these, then most likely that is what is the translation vector and hence, the Burger vector of a full dislocation for this kind of system.

So, let us draw the 1 1 1 0 0 system.

$$a < 110 > \rightarrow \frac{1}{2} < 110 > +APB + \frac{1}{2} < 110 >$$

So, here let me draw 1 0 0 and it would seem it is very simple because at the corners we and again I will have to draw 4 cells. So, at the corners this is aluminium atom and at the face centre, what is it? At the face centre we know we have nickel. So, this is nickel. So, this is 1 0 0 plane and once here the Burger vector is in this direction, so this is your a by 2.

So, from here to here it is the a by 2 1 1 0. So, now this is the shift that will take place if this is there is a extra half plane on this 1 0 0. So, everything on this plane will shift with respect to the bottom plane by this much amount. So, we also need to draw the bottom plane and what do we have on the bottom plane in the plane just next to it, ok. So, now we will again you need to go back over here to this drawing.

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

So, this is your 1 0 0 and the next layer of plane is just this one where there are only nickel atoms at the face center which in this projection will look like as if they are in the center of this particular edges. So, they are in the different layer. So, I will draw it like this.

So, the dot inside the circle represents that they are in a different plane, but they are all aluminium atoms. So, this is aluminium sorry nickel atoms, the orange one is the aluminium atom. So, now what happens when we shift the top plane by 1 1 0? So, again here what do we see? If you if the whole thing by 1 1 0, this orange atom comes to this center where it is right now red.

So, the nearest neighbour for this which is right now for this red atom, this is the nearest atom; this is also sorry the next nearest atom not the nearest. Nearest is this one. So, when nearest atom remains the same, but the next nearest for the next nearest which is in the next level and is equal to root 2 a, so this root 2 a distance atom which is the next nearest for this red atom changes. Instead of the red atom which is the nickel being the second next nearest neighbour to itself, you get aluminium being the second next nearest nearest neighbour to nickel. So, next nearest neighbour remember that term next nearest neighbour changes, it is also called as NNN.

So, first thing is when you when I say that the next nearest neighbour changes when is that this a by 2 1 1 0 is again now confirmed that it is not a lattice translation vector. So, now you can clearly see that very different from FCC. In FCC we saw that a by 2 1 1 0 is the lattice translation vector.

Second thing that it implies is that the gamma APB for 100 is less than gamma APB for 111. Why is it? Because, the nearest neighbour stacking fault or anti phase boundary will have a higher energy which is what we found in 111. On the other hand in 100 what we get is the next nearest neighbour anti phase boundary. So, this will have lower energy. So, this is another thing and this will become very important again when we talk about something that we saw earlier the anomalous behaviour.

Now, let us talk about what will happen if I use instead of a by 2 1 1 0 if I take a 1 1 0. So, what happens? Now here orange atom is shifted all the way to the orange atom; red atom is shifted to the red atom. So, everything is brought back to its original position, meaning no one will be able to figure out if any changes have taken place and therefore, we can say another thing that we can conclude from this is that a 110 is a lattice translation vector. Shortest infact, shortest lattice translation vector, we have not proved it. We have just seen by example that this is the shortest lattice translation vector which is the Burger vector for full dislocation.

Now, remember the I will be again going to introduce another term. This full dislocation is called super dislocation because compared to FCC, this is twice the Burger vector and therefore, it is as if you are talking about two dislocations put together.

And simultaneously if a by 2 110 type and I am going to say not partial dislocation, but super partials are formed, then it leads to formation of APB; anti phase boundary. So, what we see is that there is a possibility that a by 2 1 1 0 type of structure you would see. And when would you see that? When you have a super dislocation dissociating. So, let us say this is a 110 which is usually represented like 2 dislocations. So, this is a super dislocation. So, these are just terminologies somewhere at some places that you will see, but it is not much you should not get confused with that. It is also dislocation and the partials are not the same partials as you see in FCC. Therefore, there is a different name given to it as super partials. So, this can break into 1 by 2 110 which is super partial.

So, this is now represented as and there will be another 110 edge can be represented like this. And in between these two, what would we have? We will have anti phase boundary. So, whether you are talking about 111 or you are talking about 100 you will have of anti phase boundary. Of course, the energy would be different, anti phase boundary where when you are forming on 111 and when you are forming and 100 and just to remind you

which one would be lower. So, we saw that 100 has the next nearest neighbour anti phase boundary, while 111 has nearest neighbour anti phase boundary. So, 100 is the lower of these two.

It seems that we have figured out everything about super lattices and their dislocation, but we have not yet been able to see any particular reason while they should show higher strength other than that the Burger vector is higher in size that is because things become more interesting here. So, there is another interesting phenomena that can take place and which we have not yet discussed like remember in FCC.

$$\frac{a}{2} < 110 > \rightarrow \frac{a}{6} < 211 > +ISF + \frac{a}{6} < 121 >$$

And I am recalling FCC just because whenever you have on 111 1 by 2 110 dissociates into and I will say a by 2 dissociates into a by 6 211 plus stacking fault plus a by 6 121. This is I am just recalling.

So, whenever you have a 111 dislocation like this we know that something like this can happen. So, can this also happen on super lattices and the answer is yes and that makes it very very interesting. What we have now is in the FCC in the super lattices a by 2 110 and here I have missed a. So, let me write for the sake of completion. So, in here we have a by 2 translating something similar, but instead of a stacking fault we already all have a antiphase boundary over here remember. So, this is antiphase boundary added with stacking fault and it is called ISF; Intrinsic Stacking Fault.

So, ISF is so now here you had if you go back to this reaction, we saw that it had 2 such dislocations which we called super partials and those super partials can dissociate into yet another lower level of partials which is just like this one. So, you will have an inter stacking fault intrinsic stacking fault over here and then, an intrinsic stacking fault over here and two partials and in between that we will have something antiphase boundary. Now whenever you have a combination of ISF plus antiphase boundary, we term it as complex stacking fault.

So, we have so many terms now, intrinsic stacking fault, APB, CSF. So, now let us quickly let me define not in the not just the nomenclature, but what is the implication of all these three. So, let me write it over here.

$$\frac{a}{2} < 110 > \rightarrow \frac{a}{6} < 211 > +ISF + \frac{a}{6} < 121 >$$

What do you have when you have ISF occupying? So, stacking fault, it is simple stacking fault we had we have been calling; occupying an unconventional or unoccupied site. So, this is a site about site, in normal stacking sequence. What is antiphase boundary occupying a normal stacking site?

So, here it is not about the site. The stacking site you are that the atom is there is unexpected or is a normal stacking site, but not the right chemical site, but not the correct chemical site. So, this is a difference here. Chemical atoms are not the, not of concern. Here only the positions or the incorrect sites have been taken. So, that starting has been changed. In the ABP the stacking there should have been atom over there, but only instead of a b is there or instead of b a is there. So, that is APB and when both the things can happen that is what you have called what is called as complex stacking fault, a combination. So, that should make you clear about the terminologies that we are using.

$$a < 110 > \rightarrow \frac{1}{2} < 110 > +APB + \frac{1}{2} < 110 >$$

So, in summary what can happen on 111 for super lattice and remember it is about 111. Super lattice can dissociate like this and here let me a 110 a by 2. So, first level of dissociation would be like this which will lead to anti phase boundary plus a by 2 110 and usually it is represented like a super dislocation dissociating into smaller level dislocation.

Now, further this a 110, it has this a by 2 110 can further breakdown into a by 6 211 type where in between this you have the chemical stacking fault plus the antiphase boundary. So, leading to complex stacking fault plus a by 6 121. This is for this much part, ok. So, we can represent like this as this is the real partial and then, there is APB and then, this will break down. So, this can again be shown as a by 6 211 plus CSF plus a by 6 121. So, this can be shown like this, this can be shown like this. So, in all that is what all can

happen just in symbols if I have to write, it will be now this really looks a complicated thing and now it can even give rise to some complicated phenomena. What are those?

Even before that there is something that I missed let me write it down. So, you have two different types of fault, chemical stacking fault and the APB. So, what is the usual size of this? Chemical stacking fault is usually of the order of 1.5 nanometre while anti phase boundary is of the order of 15 nanometre and one more thing well is it energetically stable. So, let us also compare energy.

So, on the left hand side this is a square on the right hand side. This is a square by 6, this is a square by 6. So, a square by 6 into 4; so, this comes out to 2 by 3 a square. This is certainly smaller and hence energetically favourable. So, energetically yes, it is possible it is not just theoretical, energetically also it is possible.

And if you were to see this, how would it look like; just like we have drawn earlier the super partial dislocations. There will this is how it would look like. You will have CSF, here you will have APB, here you have another CSF. It can have a different width it need not be of the same because once they are separated, they are two different species, they are two different entities. This will be a by 6 211. So, writing the same thing just in a different form, so that you can appreciate the true picture.

Now, if you remember in FCC we said that partial dislocations always travel in pair. Why? Because, the width cannot exceed beyond a certain value. Here also we have looked that there are there is a width r 1 r 2 and the total width r. Now, this width, widths cannot be exceeded. It means that the super dislocations even after splitting must travel in pair, must glide in pair, not travel must glide in pair. Now, you have so many of these dislocations partial, 4 partial dislocations moving together and that is something that will always have to be there. What will that mean that there will always be a higher stress required for these dislocations to move and this also would mean that if there is any barrier, all the 4 partial dislocations will phase that barrier and therefore, back stress would be much higher.

So, all in all we can say that this will lead to strengthening behaviour implies strengthening of ordered, it can be in the form of precipitate or phase. So, this clearly

explains to us that why the strength of intermetallics like this which are ordered intermetallics they should be higher, but that is still not the complete picture. We earlier also asked the question about the anomalous behaviour, the anomalous ill behaviour where we saw that strength increases with temperature and then decreases with temperature. So, that is still something that needs to be explained, ok. So, that can be explained in now these words.

This is what is called as Kear-Wilsdorf Locks, ok. So, there is something called as Kear-Wilsdorf Locks and this is formed in systems which have these type of super partials and then super partials splitting further into regular partials. Now, in L12 structure 100 as well as 111 are glide planes, right, remember that, but the partials which is a by 6 211 type these are formed only on formed and glide only on 111, not on 100.

So, if somehow part of this one this dislocations were on 111 and other part was on another 111 and in between it was struck by a 100, then they will remain as it is. Let me explain what I am trying to say. So, let us say this is one of the 111 planes and this is a 100 plane. So, this is a 100 this is a 111 plane. Now, let us say here you have the partials. These are our partials in between in this you have CSF and this is connected like this over here to another set of partial CSF and here you have the APB. Now, these partials as I said earlier can only glide on 111. It cannot glide on 100.

So, it cannot come over here, this cannot go over here and you would say why not this APB this will bring them down together, it will or why will it at all go to 100. Well there is a reason for that too. You remember gamma APB 100 is lower than gamma APB 111. What it means that this antiphase boundary would like to remain on 100. So, where ever it finds an opportunity when this has not split into partials this will move on to the 100 and suddenly it goes moves back onto 111 and it has split.

So, this part is now locked, this part is now locked. So, it cannot come back together and at the same time it will not allow any dislocation to move on this plane and this plane. So, what is happening? There are so many things happening at the same time. The dislocation set I would say not pair becomes sessile or immobile. Not only that, it also does not allow other dislocations to move on these planes.

So, this is what is called as lock. Now, this has found a lock neither it can move itself it is pinned, nor it will allow other dislocations to move. So, it has it is a lock unless you put a key. What is the key? It is that you construct the two partials and then, allow them to move back onto 100 onto back on to one of the 111, but that is not going to happen because this APB prefers to lie on 100. It is very unlikely that it will like to go on the 111. It will like to stretch itself on 100. It is like want to sleep. So, it is sleeping at 100 and it does not want to you can say walking on 111. So, this is the more desired position for that.

Now, what? So, this explains another thing that these intermetallics can have very high strength, but something must be happening with temperature that strength is increasing.

So, next question is effect of temperature. With increasing temperature more cross slips take place and since they are mobile, they dissociate into partials. So, it means more and more locks are getting formed with increasing temperature. So, the effect of temperature is that more and more locks are getting formed and what is the implication of more and more locks, that strength is increasing and this is what we termed as yield stress anomaly.

So, with temperature this is increasing or leading to higher strength, but then this should happen, keep happening at higher and higher and higher temperature. Why does it break down at some point? So, at some critical temperature something must be happening. What is that is happening? The most important thing that happens at any particular critical temperature you remember order to disorder transformation, meaning now it is no more acting like L12 structure. It is only acting like a FCC structure and in FCC we know that something like this does not happen. There is no Kear-Wilsdorf Lock; meaning acts more like FCC and hence, locks not applicable anymore and this is not the only thing that is happening with increase in temperature, Peierl's stress also decreases and hence, with lower stress or with the stress requirement for movement of dislocation reduces further and further.

So, over all this leads to drop in strength with further increase in temperature. So, now you can imagine you will have, so it is increasing and this is that critical temperature beyond this it starts to drop and this critical temperature is in the range of 800 to 1000 Kelvin for a system like Ni 3 Al. And to sum up to close this session, or to to this close

this module on super alloys let us realise that L12 is not the only system, there are some other systems where you can get this kind of complex dissociation of dislocations. So, let me just write down some brief summary.

So, L1 2 is not the only system. What are the other systems? For example, B2; it forms. Now, B2 is relatively simple. It is it forms only antiphase boundary and the Burger vector here is a by 2 111. L1 2 we have seen it can form this plus CSF plus this plus APB plus this plus CSF plus this and the Burger vector here the smallest Burger vector is 112. Then there is another system D03 which forms this plus APB plus another super partial plus APB prime, ok. So, this is let me come back to that in a moment and then. So, there are two types of APB that I have listed here and there is a reason there is APB for nearest neighbour and APB. So, in the same set you are able to get two different types of antiphase boundary; one with nearest neighbour and the other which next nearest neighbour, next nearest neighbour.

And the Burger vector here is 11 a naught by 4 111. So, this is one thing and just to show that in a super alloy like, super alloy nickel based system what you have is not just Ni3 Al, it will be too brittle.

So, here you have two phases. One of them is always the more you can say softer phase. So, let us say this is the Ni 3 Al phase which is ordered all these and usually they have a structured system and this is something like a disordered Ni Al. This will be softer and if there is a dislocation moving.

So, this location would move like this, it will bow out and if the distance between the two is h, then we know that the stress required to form is this or 2 alpha G b by h. So, smaller h implies higher strength. So, the higher would be your fraction of Ni 3 l higher would be a stress required or smaller are the sub particles, you will have a smallest inter particle spacing and therefore, h will be reduced and you will lead to higher strength and then, again the temperature effect will come and so on.

So, that is all about the super lattices and next time we will talk about interaction of dislocation with other entities.

Thank you.