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

Lecture – 05 Other Defects in FCC (Twins and Frank Partial)

So, in this module we will talk of two other kind of defects that are possible in FCC materials.

So, one of them is called Frank partial. So, this is also a partial burger vector, but again this is not this is not glissile meaning it does not glide. And the other one is a very different kind, but again related to the stacking fault that we see in that FCC system. So, let start with a frank partials.

What are frank partial dislocations? Now if you remember we had the Thomson's tetrahedron like this where we had A B C and D and opposite to A at the centre we had alpha, opposite to B at the centre we had beta, opposite to C we had gamma and just below D we have delta.

Now, let us say there is a burger vector which goes from A to alpha like this or D to D delta meaning it is perpendicular to the plane A B C, but it is connecting to the point D. So, that kind of burger vector is called a frank partial dislocation. Now, which plane does this partial dislocation lie on any of the 1 1 1 plane? No it does not, you can see this is this is lying normal to one of the 1 1 1 plane and it is not lying on any of the other 1 1 1 plane. So, even without knowing the line vector we can say that it does not lie on any of the 1 1 1 vector.

So, let us look at what is the magnitude of this burger vector. So, let us say if A B C was the 1 1 1 plane. So, our burger vector is perpendicular to it so, its direction will also be 1 1 1. And therefore, it is of these kinds so the magnitude is a by three 1 1 1 and it can be represented by A alpha or B beta or C gamma or D delta. So, this is a burger vector which does not another one any other 1 1 1 direction does not lie on any of the other 1 1

1 planes, which is a fact and therefore, we can clearly say that these burger vectors let me call it frank partial does not lie in lie on any 1 1 1 plane. And hence is it glisile or sessile glisile meaning it can guide sessile meaning it cannot glide so, it is sessile.

Hence it is sessile, it cannot glide. The other partials that we were talking about, now if we have given this a name so, it is important that we give a name to the the other partials that we have been talking about so far just to keep things in perspective not can be are called which are of the type a by 6 1 1 2 Shockley partials. So, in FCC we have two kinds of partials Shockley partials which are glissile which we saw or of the form a by 6 1 1 2 and we have frank partials which are sessile and which are of the form A by 3 1 1 1.

But you one must keep in mind that they can it can still climb meaning at meaning at, high temperature this dislocation can still contribute. And just to again bring back our Thompson tetrahedron, if you remember I said this is your; from this drawing you should understand that our partial is like this.

So, if this is the 1 1 1 plane this is the burger vector from centre of this plane to the tip of this plane and that is called a frank partial dislocation. So, we will come back to this slide and like i said this can still climb and this is where it can contribute to deformation only at high temperature.

So, that was frank partial. Now the other kind of defect that is possible in FCC, they are called twin boundaries. You remember we talked about 1 1 1 plane and they have three possible layer stacking what we called as A B C A B C stacking.

So, let us visit that again here we have this 1 1 1 plane and the 3 different layers are shown in 3 different colours. So, you have one blue coloured 1 1 1 plane and you have then red coloured 1 1 1 plane and then you have a green coloured 1 1 1 plane over here. And if you start them that is when we get the A B C A B C type of stacking at that time we were looking from the 1 1 1 direction. Now, let us try to so if this is a 1 1 1 plane so, we were looking at it from top.

Now, let us try to look at it from let us say in this direction meaning what we are looking at are the packed atoms and normal to this. So, what you will see is something like this. So, you have one layer A, then you have B, then you have C again you have A again you have B and again you are C. So, you can see A B C A B C. And what is the how do we say that these are different and at what stage it becomes same so, that you will be able to identify when you put a line. So, if you put a line over here, you would see that this particular layer does not lie just on top of it is a little shifted, C is also little shifted and by the same amount when the forth layer shifted it comes back to the original position A and that is what we meant when we set ABC ABC packing.

From the top view where which was the 1 1 1, we looked at it with respect to what were the possible sites or the or the positions where it could have occupied and here we are looking a from a different perspective. So, these are the ABC planes sorry the ABC ABC stacking.

Again I am showing you ABC ABC, now what happened when we had two partials or a one dislocation splitting into two partials? So, the two partials move and we saw that somewhere that layer became or generated a stacking fault meaning in that region, you did not have ABC ABC kind of packing.

So, right now if it is ABC ABC somewhere in between that region does stacking fault was generated and how was stack generated? By displacement of a by 6 1 1 2 type of magnitude vector. So, first thing that here you can see this B and B are matching so, what we said that the atoms are shifted. Now, let us shift the A layer by a by 6 1 1 2 in this direction. Now what do you see that it has moved a little bit and then what should become the stacking. Now it should not be ABC ABC the A layer should now become B.

And similarly the other layers on top of it they should keep shifting onwards. And therefore, this will be a new type of stacking A B C B and then again it will continue. So, there is a stacking fault created which we said earlier which could be formed due to 2 partials.

So, you can say whether is 1 partial here there is another partial over here. So, this stacking has been formed let us assume because there are two partials. So, this one partial is over here, one another partial is over here and in between this is the region where we have this stacking fault generated. So, this is leading to this partial or somewhere the other gases are stacking generated. Now, this stacking fault is stable even if you have just one layer of the stacking fault it is stable and that is why a partial dislocation is possible in FCC system.

Now, let us take it further let us assume that each layer is displaced by this amount a by 6 1 1 2 in the direction 1 1 2. So, after this B layer has been pushed again C layer will be pushed and again A layer will be pushed, what do we get? We get a structure something like this. Now, what is this structure? If you look at it carefully you would see a symmetry over here. So, there is a reflection plane somewhere here and about that reflection plane, there is similar kind of atoms here and similar.

So, it would look like it has flipped onto this side let me redraw it. So, you can see it again; now you will see that this is a layer forming like this and over like this. And again here the colours have not been changed after the displacement. So, this does not represent A B layer any more, it does not represent a C layer anymore; it is just the originally B layer original C layer original a layer, now it has been moved to a very different place.

What will be the new sequence we will come to that in a moment and in fact, you should be able to call it from here, because now if this why we remember this is A, this is B, this is B. So, this is reflection if there is C this should also become B, if this is reflection then they should become A. So, this is now become this is the plane about which we are seeing a reflection. So, whatever you see over here, you would see a reflection over there and therefore, you get a structure like this this is why it is called a twin boundary. So, this it is like it is as if about this line there exists a twin whatever you have over here, you would see over there. So, this is called a twin boundary and this is an additional mode of deformation for many metals and alloys. Now, let us look at this twinning with respect to the 1 1 1 direction, now we are looking at the 1 1 1 direction 1 1 1 planes from the 1 1 1 direction. So, this is now 1 1 1 plane and we are looking this is the 1 1 1 direction.

Now, with respect to that at right now you have only three layers ABC and the other two layers should be B and A when you put one top of it. So, are the top of C, what should come if we are talking about reflection? Then there should be A B layer and you can see that the here, I have drawn it using red colour which is for the B. And it lies just above the B so this B and this B there overlapping.

Now, the next layer when I add which is a layer which is blue colour which is also the a layer. So, again you would see that this blue layer is overlapping with the blue layer on that bottom and it is indeed a twin. So, note that ABC BA arrangement which implies reflection about C layer.

So, we have a reflection or a twin around this layer and they hence we have what we call as twinning. And this is when you are deforming you have in FCC materials, there can be deformation by dislocation slips as well as because of twinning and both of them are competing phenomena. Next there would be some energy associated with twin boundaries energy associated with stacking fault energy, but we also know that both of them are being formed because of stacking fault. So, there must be some relation and there is indeed a relation. So, let us look at what is that relation.

$$E_{twin} = \frac{E_{SFE}}{2}$$

So, first let us talk about a simple stacking fault which is generated due to partial dislocations; so this is ABC ABC.

Now, over here one of these layers is moved by a by 6 1 1 2 ok, let me right it more clearly with a different pen. So, what will be the new sequence and it is let us assume that it is the top layer which is being moved. So, everything will move beyond that. So, first let us write what will happen.

So, first this these three layers remain as it is A will now become what A will become B. And now after that the sequence remain same so, after B come C after C comes A. So, this is this would be the sequence and this is where we have our stacking fault. So, this is for due to partials a stacking fault region has been generated. On the other hand let us talk about the layers that are formed when we have a twin boundary formed.

So, here also we have displacement by a by 6 1 1 2, but it is not only for one layer it is in fact, for each layer and in the end what we get is a structure like this which we have seen earlier and this will become the reflection plane. So, C beyond this it will become B beyond this it will become A so, it is a in other words you can say the sequence here becomes negative it was going ABC now it becomes CBA. So, this is what we see it is now become A.

Now, let us understand why should there be any energy associated with this, here as we said earlier that atoms of other kind are coming closer than they are comfortable with, it is this that leads to increase in energy. So, here for example, if you look at it the next nearest neighbor is B and B.

Over here the next nearest neighbor is A over here it is C. So, it is not the same type of atom or the same position of the atom. And therefore, the repulsion is weak in here, but when you come over here the repulsion becomes stronger. So, there is same type of these atoms are at the same site in the next nearest position. So, this adds to their repulsion so, let us say this is B and B this is showing that there is one only another over here. Now, there is a still one more set of atoms which should not be there, but are still there so and this is for example, C and C.

So, they are also becoming next nearest neighbor they do not want to be the next nearest neighbor, they want to be 2 atoms a part that is what means by what we mean when we say ABC ABC, but here we see that it becomes next nearest neighbor. So, it becomes C and C the energy additional energy because of next nearest neighbor coming together is delta. So, there is a delta energy here there is a delta energy over here. So, the energy of SFE we can say is equal to 2 delta.

Now, let us compare it when in that case of twin boundary, here when we look at it there is again something like this farming B and B. So, next nearest neighbours they are on the same position and they do not like that they are not happy about it there is a repulsion.

And therefore, there will be some energy associated with it which is equivalent to delta, now what about the other atoms here it is a there it is C is with it there is no problem. If we go C and a that is also again with it so, and beyond this anyways it is a regular sequence. So, there should not be any problem. So, in this neighborhood we get only one of those repulsion are the kind of you can say layers push together, which they do not want to be there in this case there is only one.

So, energy of twin boundary is equal to delta. And when if you look at it that this delta and this delta should not be different, because they are coming from the origin is same the next nearest neighbour is repulsion is what leads to this delta. And therefore, we can say that E twin is equal to E SFE by 2. So, this is an approximate relation which is found to be approximately true again as approximately we derived as approximately it is true for many of the metals and alloys. So, this is another aspect about the defect which is the twin boundary. So, we will end our lecture over here and we will see you in the next class.