Defects in Crystalline Solids (Part-II)

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Lecture – 01
Dislocation Structure in FCC

Welcome friends. So, this is part-II of the course Defects in Crystalline Solids. The name of this course is this is part-II of this course. There is also part-I of this course. And if you have not taken, you need not worry these videos are still available. And you can still go through this course you are as a registered candidate and just so that there is a continuity you can look visit the part-I course go through the videos, understand the concepts and come to part-II.

Now, about this part of the course so first what we covered in part-I of the course. In part-I of the course, we covered the fundamental aspects about two major type of defects that are found in crystalline solids one is the point defect and the other is the line defect which is dislocations. So, we looked at their fundamental aspects. What is this purpose of this part-II of this course, in the part-II of this course we will look at the advanced concepts and in particular that these line dislocations in particular type of crystal systems.

So, we already had a brief look at dislocations in FCC and BCC. But that was just a brief glimpse. We will now look take a look at it in a more detailed and complete view of the dislocations that exist in not only in FCC and BCC, but also in HCP then also in super lattices and in ionic crystals so that is one important module of this course and another module in this course is to relate this concepts to some of the important observations relate regarding properties of the materials. For example, yield point phenomena I mention this is also in the part I of the course is important property that we observe. But this is not arising out of nowhere; it is arising because of interaction between dislocations or the line defects and the point defects which is the vacancies and also solutes.

So, this is just one example. Then also you have low angle grain boundaries that you see that is that exists in materials and that is again nothing but array of dislocations. So, we will look at this and also another important aspect is strengthening effect. Now, where does strengthening take place in materials, most of the material the strengthening takes place because some way or the other dislocations are motion is getting restricted. Sometimes it may be precipitate, sometimes it may be a solute, sometimes it can be other bunch of dislocations which is called forest dislocations. So, all these together give rise to strengthening mechanism in strengthening phenomena in metals and alloys. So, we will look at these two.

So, with that we have set the contour of what will be covered in this particular course. Now, let us get started with more detailed understanding about dislocations in FCC system. So, to begin with as I mentioned even in the first part of the course that when we talk about dislocations the dislocations are usually in the first part we had a very simple view of this. So, these are planes of atoms ok. So, these are not just lines is a planes of atoms. And there is some where extra half plane and below you can call amazing plane. And this missing plane, where this extra half plane ends we call that at dislocation.

And we also had a brief glimpse at how this would manifest in FCC system. We found that the simple system is not true for FCC. What is different is that there are two missing planes instead of one. Another thing that we learned was that we did not again look at it in the last lecture we did not go in the detail, but another thing that we found was that this burger vector we usually say that burger vector is always closest packed direction. Well, in general it is true, but in here you would see that this can also dissociate into partials.

So, the two important things that we will want to look at is one that there are more than two planes instead of one and we talk about the extra half plane or extra the missing plane and that it can dissociate the dislocation can dissociate into partial. Now, with this point in view what I have done is I have prepared very nice PPT, which will give you a good understanding of what is this how this there are two missing planes and how the dislocation can dissociate into partials.

So, let us look at this. So, this is our presentation that I will show over here. What we want to show are two extra layers for planes and that partial dislocations.

So, now let us look at what is called as a ball and stick model for FCC? So, as you can see this is a cube and at the corners you have the atoms and the atoms are at the phase centers. Here the x y z axis are defined. So, this is the x; so this is y and this is the z; this is how we have defined. And you can assume that the centre lines over here at this corner.

Now, where is the 111 plane? Now, we are not talking about a family of 11 plane we are talking about particular 111, so all positive 111. So, if this is 000, so this becomes y 0, this y 1, this becomes x 1 and this becomes z 1. So, we have to connect this and ok. So, before that this is the 111 direction and in a cube 111 direction would be normal to 111 plane. So, this is your 111 plane, which is shown as blue colored. Now, here as you note that this is not the only 111 plane you could have drawn it at other locations also.

So, for example, you could have as well this is parallel we can draw it like this ok. So, this is also 111 because, if you a move it which is translated by a small vector in this direction, you would see that it overlap. So, this is also 111 and inside the same lattice this inside the same cell. And you can even draw it or there will be still parallel 111 plane which will pass through the atom over here the one where I am highlighting.

So, there are if you look very closely, you would realize that there are three different layers. And why we are calling layers because the arrangement of atoms when you look through the 111 direction is a little bit different. We always show this as the 111 plane. So, here you have so as you can see this is one line and this is another line and you have atoms which are the presenting the corner atoms and these are the phase center atoms. And with 111 particular orientation or 111 plane we can call this as 1 bar 1 0 direction, this as 0 bar 1 1 direction and this as 1 0 bar 1 direction.

So, these are these three directions if you again look at the blue one the blue plane. So, we are talking about this direction, then we are talking about this direction and then we are talking about this direction. These are the three directions shown over here. We will come back to this why I have drawn it because will need it again and again. Now, this is the ball and stick model.

Now, we can draw to in order to understand the three different layers, we can draw it also in what is called as hard sphere model. So, this is a hard sphere model. Now, you remember in FCC which is the closest packed direction, the closest packed direction is the 110 direction. And all the atoms along this 110 as you can see are touching each other.

So, in here all the atoms are touching which is how it has been drawn. So, this is 110 kind of direction this is a 110 kind of direction this is a 110 kind of direction. So, this represents our 111 plane and these are direction light a like I said this is the triangle. If you relate it with this over this triangle over here then this triangle is what is over here and it is drawn in hard sphere model. So, we are showing them touching each other which is what is expected in a FCC which is closest packed structure closest packed cubic structure. Now, here with this is the blue layer which is the first one over here. So, this is drawn as this is let us calls it layer A. So, this happens to be our layer A. How would layer B look like?

This is layer B. What is different here? Actually, if you look at it independently there is nothing different, this blue layer which is shown in red or pink is type of color or a oranges color, this is exactly same orientation. Here also you would see the triangle where the sites would represent 110 direction, but what will be different is their relative orientation with A.

Similarly for the C layer. Now, this is the C layer which is green in color. And here also the as a individual layer, the orientation of atoms are exactly same. So, the atoms are touching each other and there touching around along the 110 direction as you can see. So, this is these are your 110 direction. And if we call this as the normal of this is 111, then we can specifically say which direction is this and which direction is this as we showed in the first slide. So, the these are three different layers and like I said independently looking at it, there is no difference in any of these layers.

What is different is when you place them one over the other. Now, let us put B on top of A. Now, if you had the blue layer which was our A layer so, A layer was this blue layer. And as you can see there are different kinds of points where you can put the next layer or where the you can say truff lies where another sphere can fall into. So, these are these different truffs, but you cannot fill all the truffs, you can only fill half of the turffs, and other half truff will remain empty when you put another layer on it. So, you can put your layer either here or here. So, we can say there are two positions and one of these positions will be taken away by the B layer which is the red layer.

So, these are the ones which have been taken away. So, you can see these layers have been taken away on the alternate ones have been left empty. Whenever you have another one one layer falling onto this, this will happen that only one point one particular set will be taken or one set position will be taken. So, now we have A and B, B is on top of A.

Now, where do we put C? Now, when you put try to put C, so when you put B on top of A, there is no particular you can say preference of which one should we take, you can select any of these two. But when you come to C after putting B, then there will be a distinction between two possible sides. Now, here also you can see this is these are one set of possible sides these are another possible set of possible sides. And what is difference between these two? So, I have called one as position 1, the other as position 2. What is the difference between these two, you would see that these particular points lie in a empty region. So, the A layer are not below this. But position 2 if you look at it, there is atom A over here not atom a layer A over just below it. So, just below this is layer A.

Now, just clearly means that the two sites are very different and therefore, there will be different preference for this. Which one do you think would be energetically preferred? Now, if you put over here, what will happen is that A layer and C layer will be one on top of each other, very close to each other and therefore, there will be a lot of repulsion. But, if you put C layer in this vacant region, then that repulsion would be minimized. And therefore, clearly this position 1 would be preferred in terms of minimizing the repulsion.

So, let us put C layer on top of it. Now, this is what we can call as the ABC layer that is found in FCC. And it is called ABCABC stacking. So, ABC another layer will come just on top of ABC. So, this will give you the what is called as ABCABC stacking of FCC.

Now, if we have selected position 2, how would it look like, the green atom would fall right on top of blue atom and it will look like this. So, this will be green on top of blue and so you are able to see only two layers. The B layer which is reddish in color and the A or C layer which are same. So, this is called ABAB type of packing because now we have only two different positions here A and B. The third again goes on two or on top of A. And actually there are crystal systems where you see this and it is HCP systems. In

HCP also you can get ABAB type of packing you know the 00001 direction you get ABAB type of packing in HCP. So, this is the HCP type of system.

Now, let us come back to our so now les come back to our ABC layer of FCC. Now, where is our 110 direction? So, like I said these are our 110 direction and these are what these are if you look at just half of it, this will become your burger vector. So, ideally these are your burger vectors. Now, if I take a edge dislocation with this as the burger vector, then what should be the orientation of the line direction, if this is the burger vector that of the dislocation that I have selected for a edge dislocation, then the line vector must be perpendicular to this and the line vector must line must lie something like this.

If this is the dislocation line, when where is the extra half plane or the missing plane, the missing plane is lying just above it ok. So, we somewhere over there, the missing plane will stop and over and above it there will be a missing plane. So, this will be the let us say this is just the line and therefore, the missing layer stops here or the extra half plane which is below it just ends over here. So, this is our dislocation line and where our missing plane and so or the extra half plane ends.

Now, how will it look like? This is how it looks like? So, this there is one layer of missing atom one atom here, one atom here, here this. So, one layer of atom has been moved, but then what you would see is that this is not really one layer of atom that is missing, you connect straight lines all these connecting points there the atoms could have lied this, this, this and similarly over here. So, this forms one set of planes and this forms one set of parallel plane.

So, earlier our convection that there are two missing half planes is now proved over here. This is our burger vector and this is where the extra missing a layer of planes are missing and it forms two layers, one along this line and one long this line. So, there are two layers of missing plane. So, one thing we can clearly see that now. And this forms one whole dislocation.

Now, let us come to another aspect which is the partial dislocation. So, here what do you see here you see that this dislocation this is what the burger vector is. And the atoms would move like to move from here to here and then it will have actually moved one atomic plane which is how the dislocations glide. So, I really this is the burger vector that it should follow. But then what you would see is that all though this is the shortest vector, but in terms of the lattice parameter, but there is still another shorter vector. And if you find the magnitude of this, you can very clearly show showed that this would be like this of the type a by 6 112. We will come to that again in one a little bit later. So, this is your another partial, not partial, we will not call it partial will come to will define it later on, but this is the I am just showing that this is another possibility.

So, this is the original vector and there is a possibility that instead of going directly the atoms going move over here and then move over here. Let us see how it does that. So, here you see the atoms have moved from in that position to this position so, this, sorry, this position to this position. And from here they can again move over here. So, the whole dislocation line has moved from over here to over here.

So, let us come back again over here. So, this is we said there is two missing at planes of atoms and ideally this dislocation would like to move along the 110 direction, but it so happens that in this particular configuration, there is even or shorter route possible. Now, we have to find out will see later on, but right not right now we will show that a by 6 112 path is energetically favored and that is if you look at the energy relation between the original burger vector and the two smaller burger vectors, then the two small some of the two smaller burger vector energy comes out to be smaller. So, this would be a possible feasible path. And geometrically also we see that this is feasible so, yes this does happened.

So, as here also have shown that 1 by 6 or a by 6 112 direction are the smaller green arrows. In usually why would you not prefer it or why this would have any kind of you can say resistance, this is because the third when you go from in this particular fashion, when you go moved from this place to this place, what actually has happened is that the atoms have moved away from position 1 to position 2. So, the C layer this extra half plane that we are talking about is not lying on the C position which was the position 1, but it is now lying on position 2 which is right on top of blue.

Now, you can see clearly here this is the green atom and just below it is the blue atom; this is the green atom, just below is the blue atom; this the green atom and just below it is the blue atom. Similarly, all these atoms that you see over here are lying on position 2 which is you can say is not the preferred stacking sequence. So, now it has become ABAB in this A. So, there is no C position in this for this particular layer.

On the other hand, your remaining system, it is still following that ABCABC. So, the other part is not concerned about how they are oriented in between. So, the only resistance to forming this partials would be the stacking fault energy. And we will see that in more detail. So, we have the this full dislocation over here, and we have moved just one layer. And when you move as another layer, when you have moved just one layer of atom, what you see is that the two lines that we drew can now be separated into two parts. One is to the left of this extra layer, and the other is to the right of this extra layer.

So, now in a way what you are calling is to place together for the extra half plane have now dissociated, they have become into come into two parts. And this is what we can define as partial dislocation. So, the burger vector for this partial dislocation would be this one. Similarly, the burger vector for this partial dislocation would be this one. And when this to come together when then we have this as the burger vector of the full dislocation.

So, here I showed that it can move back and then you have completely displays the extra half plane or the missing plane layer by one atomic distance. So, this is what you would ideally expect, but now let us get back to this position and where there is these two partial dislocations are over here. Now, let us assume that there is some amount of repulsion between these two. Now, this can behave like a like two different dislocations right. They are now they can be treated as independent dislocations and since they have almost they have some components similar to each other. So, there will be net repulsion. And this is one dislocation, this is another dislocation and they will try to repel each other.

So, what will that repulsion do that repulsion would lead to something like this, meaning what has happened what changed here.

There is another layer of atom that has moved so this line as; this line as moved independently now it is not connected with this, its movement is no more related with the left part. The right one has just move to one step right and it has allowed another layer of atoms to move over here. So, you have you can see that there is a dislocation line over here there is a dislocation line over here. And in between these you have the region which is if as you remember does not follow the desired sequence of atoms which is ABCABC. It has ABA type of sequence. So, this region can be called as stacking fault region.

And onto the left of this, we have the perfect crystal; onto the right of it, we have the perfect crystal. So, a full dislocation line has got dissociated into two partials and assuming that there is a net repulsion which will see later on when we come to the mathematics of it. Assuming that there is a net repulsion, these will keep moving away.

And they will keep moving away and there will be a stacking fault region which will have some energy raised. So, this is a stacking fault region meaning there is a 2D defect along with this line defect that you see two line defects over here or 2D defect is being created in between this which is called as stacking fault region. And there will be some energy associated with this stacking fault region.

Now, how far these dislocations the partial dislocations move that will determine how long this stacking fault region is. And the larger the stacking fault region is larger would be the energy. So, in here what is what will happen is that there is a net repulsion acting which is trying to pull out the dislocations apart. And there is stacking fault energy being created when the dislocations are moving apart and therefore that will try to keep this to the minimum. And therefore, there will be a balance created which would lead to equilibrium thickness or width of this stacking fault region. We will come back to this in the later slides.

So, in these particular slides what we have shown so far is that there are two extra half planes. And that these two extra half planes act when you were they can move apart and they can form partial. So, both these things we started to prove show two things and the now we see that those two things are related. What are those two things that a full dislocation in FCC the edge dislocation contains not one extra half plane, but two extra half plane and then second part that these two that it can form partial dislocations. Now, we see that these are because of these two extra half planes. The two extra half planes can move a part and therefore and they can keep moving apart and they will act as independent dislocation or the extra or the partial dislocation. So, I will end this over here and we will come back to mathematics of understanding the stacking fault energy, the equilibrium stacking fault energy width of this dislocation.

Thanks.