Defects in Crystalline Solids (Part-II)

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Lecture - 07
Soft core and Hard core for Screw Dislocation in BCC

So, in this module as I promised earlier we will be talking about Dislocations and particularly Screw dislocations.

Again screw dislocations are something very interesting in a BCC system. So, here will look at the Dislocation core of screw dislocations.

Now, in this is a BCC system and the rows that lines that you see our along 1 1 1 direction. So, in a Screw dislocation for a BCC, we all know that we will we should have burger vector as well as line vector should be along 1 1 1 direction and if we take this as the centre or the origin, so this then we will have these lines representing x the 1 1 1 direction. So, these are all representing sorry I mean 1 1 1 directions, now if you were to look at along any of this 1 1 1 direction.

So, let us say you are looking at 1 1 1 along stretching extending this and let us say your. So, as if a person is looking towards the 1 1 1 direction, so this is a 1 1 1 plane meaning we have 1 1 1 plane like this. Now, when you have something like this you would see certain rows. So, all the atoms would lie in rows like this and all that rows can be actually designated as 3 different kinds so we have designated it here as A B and C. Now in each of the row the characteristics is same, each of these row the atom spacing is apart by a by 2 1 1 1 ok. But what is different between A B and C and what is common between CCC or BBB is that the atoms in these layers are in the same plane and how much are the different, so if you go from A to B then it will be one-third of this burger vector.

So, there will be know this is burger vector, so A to B the difference between the atoms along this direction along the 1 1 1 direction you have a spacing of equal to A by 6 1 1 1.

Similarly when you go from B to C and similarly when you go from C to A. But when you look at B atoms all the B atoms are in the same plane, when you look at C atoms all the C atoms are in 1 plane and when you look at A atoms then all the atoms here we have only shown one row of A atom. But there will be other for example, here will be one a there will be another A and those atoms will be in the same row.

Now here again it is we have tried to show the same thing in this BCC. So, here you have 4 cells in adjacent to each other and here what you are looking is this is the B row this will become the C row and you can see the if you are looking from 1 1 1 direction, then this plane and this atom would be in the same plane and so on and if you are talking about A row. So, all these are atoms are here the A row and this will form this will be A row this will be A row this will be A row and so on.

So, what we are trying to say is that when you are looking in the 1 1 1 direction there are 3 different kinds of rows A B and C and we have described what is the difference, that the difference is the similarity first is that the burger vector on along this is the same which is a b by 2 1 1 1 and therefore the atoms spacing is equal to a by 2 111 that is the shortest lattice vector. But when we go from the plane A to plane B the atoms are displaced by this much amount, which is 1 by 3 of burger vector equal to a by 6 1 1 1. Similarly B to C there will be a displacement of b by 3 equal to a by 6 1 1 1 and so on because of this what you would see here is that now you have A B and C.

So, let us say A is the layer where you have the lowest level of atom next 1 by 3 b this is another 1 by 3 b and then again another 1 by 3 b you come back to A. So, what this will this is forming is a helical structure. Similarly if you look at this one this is forming also helical structure only in the opposite direction, so this was in the clockwise direction which is shown in green. So, this is clockwise A B and C A B and C this is clockwise and this maroon one are in the anticlockwise direction so A B and C; A B and C. Now this leads to what is called water called as Hard core and Soft core for the screw dislocations. Let us try to understand what are hard cores and soft cores.

So, we talked about triangles over here, so here we talked about triangles A B and C, so let us look at one of the triangles where the rotation of the atoms is clockwise. Now let us try to draw it in a 3 dimension so how would it look like. So, let me try draw it from a

little bit bottom, so this is 1 row of atom, this is another row of atom, this is another row of atom and this is A layer this is B layer this is C. So, let us say the atom is over here and here it will be one-third shifted in the along the 1 1 1 direction.

So, you remember this is will draw it again. So, this is B, this is C and again this is A, so this was also A and like I said from the previous light what should be this distance this is equal to burger vector, which is equal to a by 2 1 1 1 this is what we talked about, this burger vector should be equal to b y equal to a by 2 1 1 1 spacing of atoms in each row. So, this is a row and here the atom spacing is a by 2 1 1 1, but when we look from with respect to this plane the difference between the atoms in this layer and this layer is 1 by 3 b which is equal to a by 6 1 1 1 and this is again a by 1 by 3 b. So, this total becomes 2 by 3 b and overall what you get is a clockwise structure like this. So, this is you can say inherent screw not dislocation, but inherent screw in BCC.

Now, let us say that actually another screw dislocation with clockwise orientation tries to add with it. So, there is an another screw dislocation and over there the structure would be very similar you will have, so everything is similar and here also this is clockwise and what we get. So, now look at let us look at this one first, here this is 1 by 3 b this is also 1 by 3 b. So, the displacement in this direction is 1 by 3 this displacement in this direction is 1 by 3. So, the displacement in the B row will now become 2 by 3 b. So, this will be now somewhere over here, over here the displacement was 2 by 3 here the displacement was 2 by 3 b, so it becomes 4 by 3 b which is equivalent to saying equal to 1 by 3 b.

So, this will become 1 by 3 b and this is b and this is b 2 b so it is equal to saying 0, so it remains at its position, relative positions we are talking about the relative displacement of atoms when there is a inherent screw and there is actual screw dislocation coming in and adding on to it, so how the displacement looks like.

So, now what happens here? Now you see this is 0 this is 1 by 3 b this is 2 by 3 b and there will be let me first write it. So, this is 4 equal to 1 b and therefore what we get is screw dislocation possible it is still a screw dislocation and what is more important. So, let me write down first here this is a screw dislocation. What is more important here is that the relative positions of A B C remains same, meaning A and B layer are still 1 by 3 b apart A and C are still 1 by 3 b apart. So, the relative positions and of A B C remains

same and what does that mean it implies that the energy of this core would be lower and therefore this can be termed as soft core.

Now, let us look at another possibility, again we will start from a inherent screw, so will have to re draw this structure. So, we have A here there another A this is B and this is C. So we are only considering the clockwise triangle in the BCC, the other thing also you can take and you will see that you will get similar result, not similar in fact the same thing in the inverse order.

Now here we are adding but this time instead of changing the inherent screw in the BCC we will change the screw dislocation. So, earlier with that screw dislocation that we added was a clockwise, now what will do is we will add a anticlockwise screw dislocation. So, let A B at the same place because, we are talking about relative position it will not make a difference, so will take. So, over here will put this here.

So, this is so here you can see this is a clockwise, I will have to draw it over here. So, this was also clockwise and we ended with the anticlockwise, here we start with clockwise and adding a dislocation which is anti clockwise and then what we want to see what happens. So, first let me so these are the 3 rows, now let us look at it will start with B, so over here this b is at 1 by 3 and here it is a 2 by 3 b, here this is 2 by 3 b and this is 1 by 3 b, b being the small weaving the burger vector and this is the whole thing is the b the burger vector. So, if we add 1 by 3 b to 2 by 3 b what do we get? We get 1 full b.

So, the next layer there is one layer here this another layer is over here, we add 1 by 3 b to 2 by 3 b we get 1 layer here 1 layer over here. So, this is B this is B and A is so will keep A at the same place now what do we get we get a configuration which is very funny in fact this is like this and this is like this. So, what is happening? A B and C, the layers which were supposed to be 1 by 3 plane apart have now all been pan caked on to 1 plane. So, this is the so what we are saying is that the relative positions have changed, implies this is a hard core.

So, this is what we mean by soft core and hard core. Here soft core meaning that this is so you have the inherent screw dislocation and screw dislocation added when they are of the same size and you get a structure which is anti clockwise, but what is maintained is the relative spacing between the different layers. So, they are still maintained and therefore you can expect it to be lower energy. On the other hand when you have a

clockwise inherent screw in the BCC adding to a anticlockwise screw dislocation we get a structure where A B C layers get pancake and there is no the relative positioning of the atoms has been messed up. So, this energy will be much higher and therefore this is termed as hard core and this dislocation would not like to be in this.

Now, instead of taking the clockwise screwed inherent structure we could have as well taken anticlockwise and then we could have done the same thing. So, what you would have found that anticlockwise likes to go with anticlockwise screw dislocation. But the anticlockwise inherent structure does not want to go with clockwise dislocation, meaning opposite science are not appreciated they do not want to go together they end up creating a hard core. So, this is the message that the same type of screwness in the dislocation as well as the inherent structure is light and this is what we mean by hard core and soft core, so little bit more about the hard core and the soft core.

Now, here again I have drawn the same thing and here you can see that there are the this is right now what I am showing you is the inherent screwness or inherent structure of the BCC. So, when I say clockwise I am talking only right now only talking about the inherent screwness that we saw thus helical structure that is, also there is a clockwise all the green ones are clockwise and the and the moron once are anticlockwise. Now we also said that a dislocation of the same kind would like to go here, so a dislocation which is of this type would like to go if you can see these are the grey regions.

So, all this grey regions this will be the grey regions will be soft core and the white regions would be hard cores. Now when we talk about another dislocation of dislocation of another sign which is anticlockwise, so this will like to go where they have already (Refer Time: 18:02) structure like this and therefore it will like to go into the white region is soft core and grey region is hard core.

So, if you have a dislocation like this you want to sit over here and from here you would want to jump to here to here, here, here or in this, in this. So, there are 6 different possible directions 1 2 3 4 5 6 ok, but in between all of those you see there is a grey region for this dislocation. So, there is kind of a energy barrier in between the dislocations or form movement. So, whether you are talking now even if you talk about this clockwise dislocation which is over here, so let us say it is here in this is the soft

core for this and it may want it will want to go here, it will want to go here it will want to go here it will want to go here and here and there will also be over here. But in between you would see there is a region of hard core for this type of dislocations. Now when we are looking at it like I said this is a 1 1 1 direction, we are looking in the 1 1 1 direction and over here this is your this is your bar 2 1 1 direction meaning this planes are your 2 1 1, 1 1 2 type of planes and this is your 0 1 bar 1 direction.

So, if we talk about planes so this is the plane should be oriented like this, for one of the and there are 3 possible planes. So, if we talk about this 1, so let me select another colour which will make it easier; these are 3 different 1 1 2 planes, all these orange colour that you see over here are the 1 1 2 planes. What about the 1 1 0 planes? The 1 1 0 these are the 1 0 planes you can see this is the directions. So, this will be the plane this is 1 of the 1 1 1 0 plane which is 0 power 1 bar 1 and these are the other 3.

Now if you look at those screw dislocation this 1 or this 1, let us say there is 1 screw dislocation here another is here for them there are 6 possible directions in 0 1 1. Now, including the positive and negative similarly 6 possible directions in 1 1 2 direction including the positive and negative. So, as such a screw dislocation would like to move.

$$\tau_{PN} = \frac{2G}{(1-\upsilon)} \exp\left(\frac{-2\Pi w}{b}\right)$$

So, screw dislocation will be a long line and 1 section each of this section if you look at a small section it has 6 possible possibilities in 1 1 0 directions 1 1 0 planes and 6 possibilities of 1 1 2 planes. So, screw dislocation has 6 possible 1 1 0 for a planes and I include the negative ones otherwise you have only 3 and 6 possible and because of this there is this creates because, different sections will want and the different sections want to move on to different directions. Different directions planes basically which plane to select and this leads to you can say pinning and also formation of prismatic look which will show in a moment. But before that some more properties about the dislocation based on it is core structure.

We already said that there is no spreading on 1 1 0 or 1 1 2 plane, what it implies what it implies, if you go if you remember in the tau PN we had something called as tau PN is which is the pearl Navarro stress it is proportional to do 2 G 1 minus nu exp minus 2 pi

w, with w was the spreading by b. So, more the spreading smallest the stress, if there is no spreading it implies tau PN is very large.

So, this also implies that screw dislocations are not very mobile; this is coming directly from the pearl Navarro stress relation. On the other hand if you look at non screw dislocations they are very mobile and what will happen is that there are screw dislocations which are not mobile. So, in the process they will wherever they will leave it even a small amount of screw dislocation it will remain like this and in the process screw dislocation length will keep on extending. Because, it cannot move as freely as the non screw dislocations and therefore it will it is length will keep on increasing and this creates long sections.

Now, if you look at a BCC material, if you have to look at the dislocation structure what you would see is that it is now come will fully dominated even a small amount of after deformation it is fully dominated by screw dislocations, because the non screw dislocations are very mobile, they can keep interacting reacting and in the process they are stretching the length of screw dislocation, so everywhere there are screw dislocations. So screwed the plastic deformation will now be controlled by screw dislocation, let me add another slide here to draw the diagram that I am trying to say explain how this.

So, let us say you have screw dislocation like this, let me redraw it. So, there is a small section of screw dislocation let us say this is the edge dislocation path. So, this is along 1 1 1, now this if this is the 1 1 1 this is the screw dislocation, this is the non screw dislocation. Now this is mobile so this can keep moving and when it moves what will happen is that this part will become more longer screw dislocation.

So, this non screw dislocation reaches there, there is again extends over here and this comes over here and this can keep on moving and in the process what you see there is non screw dislocation remains almost same. But this is the screw dislocation and it is length has increased and like we said that these are not very mobile.

So, they will stick to their place and in fact you will see them as straight lines many a times. Now even when they move they will move, there are many possible directions, so

let us say this is because of their limited motion they will also generate prismatic loop, so this is what I am trying to show over here. So, let us say this is the screw dislocation and a part of the edge dislocation over here another dislocation over here and then again this is the screw dislocation type so this is 1 1 1.

So, this is the screw dislocation this is screw dislocation this is the non screw dislocation in this is again non screw this is screw and so let us say there it has moved onto another plane like that and there is another segment which is in the different plane will I will try to draw it again with another arrow. So, this over here these are your now let me so this is screw, this is screw, this is screw and if it were there here screw, screw. So, this is the screw dislocation and what we have here how it is moving is like this, this one is moving in this plane then it has moved to this plane and then again it is moving back to this plane; over here this is jumping then moving here and then moving here.

Now, what will happen? Next what would you expect here is something like this. So, this is non screw dislocation this is mobile this can come here like this, this can come here this can keep moving like this, this can keep moving like this and after sometime what you may end up with is like this. So, this is here and the whole screw dislocation is now over here, it moved like I said part of it moved in through 1 direction the other part move through other directions. But eventually they are all on now one plane along 1 line and in the process these parts which we saw over here they have now move together to form a loop and these are all non screw dislocation meaning a prismatic loop.

So, there have been observations of structures like this where you see in BCC particular you would see long screw dislocations and by side of them you would see prismatic loops. So, this is what we have covered a lot about the dislocations, particularly about the screw dislocation which make them very different from FCC. So, we will end our study or understanding about dislocation about dislocations in BCC and next time when we meet will start about another system which is HCP.