Defects in Crystalline Solids (Part-II)

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Lecture - 10
Dislocation Structure in Ionic Crystal

So welcome back and like I promised we will come to a bit more advanced. So, we started with very simple systems like FCC VCC, it is I mean relatively simple we have seen that they are not really as simple as we thought it to be. Then we moved on to a more complex system like HCP. And there of course, understanding is still very limited and we, but we look saw that many other things are similar to FCC system. Now we come to not a metallic system, but a ionic system.

So, now we will be talking about Dislocations in Ionic Crystals. Now why am I baking making a big deal about ionic crystals? It is because there are electron charges electronic charges associated with each atom. Now, depending on the type of dislocation and on the plane at which it is moving, there be a net no charge or there may be net some charge on the dislocation. Similarly the jocks are the kings that form they will also may be charged or neutral depending on what are the particular direction and place. So, just to give you can say a taste of how it can be different, we are going into this topic of dislocations in ionic crystals. And one of the simplest system that we can think about is NaCl. Now what is the NaCl system like or the rock salt that is the structure that is commonly called? Now in this rock salt structure it is two into what is called as two interpenetrating FCC structure.

So, let us look at how it how it is really looks like. So, I will have to pay some special attention in drawing this because it is not a very simple system to draw. So, this is a system where we have what you can see right now I have not drawn the atom. So, let me now put the atoms over here. So, what I will do is I will put Na with pink and this one is complicated not because that structure is complicated just because I am try there are too many atoms in one cell that I am trying to draw. So, if you look at just the sodium atom positions, you should be able to realize that this is nothing, but a simple FCC system.

So, there is atom over here. So, I have drawn it all the corner atoms and the centre atom so this is all over. So, I have all the corner atoms here, I have all the corner atoms here face centre over here and on the back face this is another corner atom that I was missing this is another face centre atom missing. And again here there is another atom that is missing and like I said these are all sodium atom. And what is it forming? If you look only at the structure of sodium atom it is FCC ok.

So, now let me draw the chlorine positions. And where are the chlorine atoms? So, the chlorine atoms are over here. Now just looking at this you may not be able to realize, but when you draw 2-3 cells, you would see that chlorine atom also forms a FCC structure. So, if you look at this face what you see is you can say this is the beginning of half cell of the chlorine at chlorine atom. So, this is the face all the corner atoms are occupied by chlorine face centre is also occupied by chlorine. And then again this is another face over here. And here this is the these are the corner atom this is a face centred atoms. And if you had drawn another layer you would be able to see that this is actually the chlorine atom is also FCC.

So, this is what is called as inter. So, it turned out to be decent diagram. So, it is interpenetrating FCC structure. And like I said why is it so important? Because here Na is charged plus and similarly your chlorine is charged like minus and because it is a interpenetration penetrating system it is not the usual FCC slip system.

So, what is the slip system here? The slip planes for this one or 1 1 0 1 0 0 and occasionally if it were a slip if it were FCC, then the slip planes would have been 1 1 1. But here this is not the case these are the preferred slip planes. And in some cases you may actually end up seeing 1 1 1 slip planes and even 1 1 2 slip planes. And what is the shortest latest lattice vector well that we cannot change that is still 1 by 2 1 1 0.

So this is again although we are using shortest lattice vector as a by 2 1 1 0. But then that is what we have not explicitly mentioned as you will see that there is not just one extra half plane, there are two extra half planes. So, what do you mean by that let us see. So, again some more drawing over here.

So, let me start with structure like this. So, this is our 0 0 1 plane like we said that 0 0 1 plane is one of the possible slip systems slip planes. So, this is a 0 0 1 plane and the directions if you want to look at it, this will be your 1 1 0 in this direction and 1 bar 1 0 in this direction. So, this is this can be our one of your burger vector or this can be a burger vector. But right now we are assuming this is your burger vector in this direction. So, there is what we are seeing is that there are alternating layers of atoms with opposite signs.

So, now, you can see already that this is the structure is unique from what we have seen earlier. And I am trying only a small part of it. So, that I can show you the structure of the edge core there will be it does not mean that beyond is there are no atoms, there are atoms beyond that. And with similar charge I am just drawing a small section or some region close to the dislocation core and moreover this way it becomes a little bit easier to draw the system. So, that is another advantage when I am drawing it like this I easier to remember where do these atoms lie.

Now, you see this is your again I will have to show you the extra where does the extra half planes lie. So, what you see and I will delete these lines to make it easier to understand now. So, what you see over here? This is the structure. Now what you see there are because there are charges you see there are three planes here and on the bottom there is only one plane. So, here two planes with opposite charges are missing on the down. So, one thing to realize is that edge dislocation is now clearly different from a non ionic system in that you have two plane missing.

Overall structure if you look at it is like a simple cubic, but still a not a real FCC it once you have inter penetrated then each of them the total system is acting like a simple cubic. And in that sense you have two layers missing even though it is a simple cubic system. So, this is your dislocation core and as you can see this is your where this is where your edge dislocation. We can draw it like this and the burger vector would be drawn like this which is 1 1 0 a by 2 1 1 0.

So, what are the things that we note here? One that ok; I need to draw another pictures. So, I will not right here I will quickly mention at this point. What we are noting is that two planes with opposite charges missing. And now if you look at it may seem at this stage that the core has a net charge, but then what happens in the layer below it if you go

back to this one in this is your so, what we have drawn is a 1 0 0. So, these are the alternating layers. So, if behind this that is the opposite charge. So, behind each electron with behind each atom the charge the there is a atom of opposite type and therefore, opposite charge. And intern; that means, that what you will get if you go one layer behind it would be something like this. Now again I will have to so these are guidelines that I am drawing. So, that I can so this time I will start with minus over here, I will have plus just before below this.

So, below this plus is minus below this minus is plus and so on. So, that is what I am trying to draw here. So, this is the layer just one atom below this. Now what do you see here? Again we see this is your dislocation core and I will draw these guidelines for you to be able to appreciate. So, the burger vector still remains the same which is our a by 2 1 1 0.

And what has happened the dislocation core the charge of the dislocation cores core has reversed here it was minus here it is plus. So, this is one of the effects that alternating layers consist of alternating charges. Now what so here I have drawn it for 0 0 1 and I am not going to go in detail like I said earlier. What I will just note down a few important things about the dislocations in ionic system is that.

If you are looking at if you if dislocation was on plane 1 0 0 so, the glide plane here is assuming that 1 0 0 here. We are assuming the glide plane to be 1 1 0 because we have said this is also one of the possible glide planes. But then the other glide plane and preferred glide plane is also 1 0 0.

So, if the dislocation was on plane 1 0 0 glide plane I must say ions at bottom of extra half plane would be of same sign meaning that whole row of atom would be of same sign. Now when this is the case it implies that these this type of dislocation can interact with charged particles few more things about the edge dislocation.

For edge dislocation gliding on 1 bar 1 0 slip which is this 1. So, this is the plane is 1 bar 1 0 the burger vector is 1 1 0. So, the when the edge dislocation is gliding on a plane like this the one that I just drew then there are few more things we can say no displacement. If the line the whole the dislocation core is not moving along the line it means that there

will be no net change in the charge or so; the atoms of opposite charges would basically not come here in contact with each other or similarly ionized or charged particle will not come closer than it is equilibrium position to the dislocation core.

So, there no displacement along line which is not which is what is the case if you are looking just at the dislocation core. If you move along those line the atoms are there will be no basically displacement. And when there is no displacement it means that there is no change in the charge.

Now another thing that you will notice that if this is the dislocation the dislocation line is threw in the perpendicular to the plane. Now if this dislocation line moves over here that there is same charge from here to here to here to here. And therefore, if this dislocation moves over this tries to small kink is formed in this direction. Then that kink will not have any adverse or any kind of repulsive forces because of the charges because the charges are of the same kind whether it is here or here or here. So, where even a small kink is found that kink will be will have the similar charge as was for the original dislocation.

So, this is also what is what I am trying to say that there is no displacement. Actually I should say displacement of the line of charge along line implies no effective charge of emergent point the point which is moving ahead which we implies that kinks have no charge where the we discussed what are jogs in kinks in part 1. So, kinks have no effective charge.

Now another aspect this is about jogs now when we are talking about jogs elementary jogs will not be charged in neutral elementary meaning the 1 atom height if you look at it. So, again you can go back here the charges are of different color. So, here it is plus here it is minus. So, if you have play jog which is one atom height then it is charge changes as if you keep moving. So, odd number of steps are there in the jog or odd number of layers in the jog that it will have it will not be charged neutral, but if it is even number then it will be charged neutral.

So, that is why I am writing elementary jogs will not be charged neutral and implies that it may attract or repel electro statically. So, this is about the edge dislocations. Now just

again without going into the details just because we have started this topic let me write down a few things about screw dislocations.

Now, screw dislocations if it is moving on a 1 1 0 type of plane. And if it has a burger vector 1 1 0, then it cannot or it cannot cross slip onto any other 1 1 0 plane can you think of why. So, what I am saying is that if it is on a 1 1 0 plane with a burger vector also of the 1 1 0 type not exactly the same it cannot be. So, if you have a screw dislocation of that kind then it cannot cross slip onto another 1 1 0 plane and the reason is that particular burger vector of 1 1 0 type is can be contained on.

Or that particular burger vector can only be obtained on one 1 1 0 plane it cannot have more than 1 1 1 0 plane. So, that is because of 1 1 0 vector can be contained on only 1 1 1 0 type plane another important aspect about screw dislocation; so, displays if you look at the core of the screw dislocation along 1 1 0. So, let us look at 1 1 0 direction which is which will be the line directions. So, if we are talking about here.

So, this is 1 1 0 so this is the 1 1 0 direction. Now what you see all the charges all the atoms are of same type whether it is Na in this particular case it will be Cl again it will be Na. So, it is of the same charge. So, core of screw dislocation has same charge along the length.

It implies that displacement parallel to burger vector results in no effective change of charges. Or no relative change in position of ions. So, these are some important aspects and as you can see that when you are talking about ionic system. Just because it is ionic and we have not even gone into the complexity of stacking fault or that what is called as chemical stacking fault.

So, just looking at charges we can see that there are so many complication arising. So, many different type of interaction can arise. So, that is just to give you a glimpse of how a dislocation can be inside ionic system. So, that is all we will cover about the dislocation in ionic system. Next time we will come and talk about a more interesting system which is dislocations in super lattices.

Thank you.