**Defects in Crystalline Solids (Part-II)**
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**Lecture - 09**
**Burger Vector and Partial Dislocation in HCP**

Ok so we were discussing about SCP system and their slip systems. So, we started with looking at how to give index indices to their drip planes and direction. Then I showed you some examples and then I listed out some of the possible slip systems in HCP.

One of the things that; I want to add to the slip systems that we discussed here is how many independent system each of them is. So, here if you look at it, it is 0001 plane. So, it is only one plane it is not a family of plane and one direction. This direction the three possible directions, but then if you look at independent systems there are only 2 independent systems. So, we are talking about. So, for the basal plane we have only 2. Similarly for prismatic we get only 2 and pyramidal and basal pyramidal together they give 4. This is for the a type of burger vector slip system.

The other one we talked about was the c plus a system and over there if you look you will have another few sets of possible slip systems. So, here you have the 4 slip systems over here for the 3 planes over here. And so there are quite a bit of possible slip systems that are available in HCP system. However, not all of them are active at all the times and if you look at the (Refer Time: 02:01) stress relation then you would find that only the basal slip system is the most preferred one, why?

Because if you go from there we know that the planes which are furthest apart they should be the most they should give you the lowest shear stress the critical resolved shear stress and for the HCP although in the third direction c there is no direct relation between c and a. As you will see that if it is ideal case what will explain what is ideal case then in the ideal case the plaining plane systems are far apart. And when the and those planes are further than the ideal system then again the basal slip becomes much more preferred.

But before that there is one more thing that I want to let you know that there is still another part type of slip system theoretically possible where you have only c type of burger vector. But unfortunately there is this does not exist on any plane. So, you will write it as like this and this is not there is no independent slip system meaning this does not exist. So, theoretically it is there, but practically we do not see anything like this.

Now, the next thing is like I said what is a ideal hexagonal system. Like I said that you remember in the beginning I said that in the HCP it is not really hexagon their unit cell is not hexagon it is rhombus. We have atoms over here and in this these are the basal place. But in between also there is one layer and there is atom over there too. So, if you draw a middle line level mid plane somewhere over here which is this mid plane will be called the b type of layer.

So, these are your a layer and this is your b layer and in this b layer somewhere over here in only. So, if you divide it there will be two triangles and one of these triangles will contain this b atom. So, this forms B layer and these layers form A B and we all know and I have already said again and again that HCP is AB AB type of packing ok. So, now, coming back to this now let us look at these four atoms 1 2 3 4. Now if you look at it this is at the centroid of the triangle over here. So, this when you connect what this forms is a tetrahedron and you can clearly see that all of them are equilateral triangle.

And therefore, if this is a all of this length would be a. So, it is a tetrahedron with edge length equal to a. And again let me remind you this is when we are talking about ideal ok. Now in non ideal case this is your c direction and this is a direction there is no relation there is no way to exactly define what should be the relation between c and a. What we are looking at right now is c by a ratio when it is a ideal condition. So, trying to find c by a for ideal.

So, if you look at it this height which will be equal to c by 2 you can very easily show that this is equal to root 2 a by root 2 by 3 times a which is nothing, but half of c. So, this is equal to c by 2 which implies that c by a ideal. Now this whatever we are describing as ideal is also a close packed structure meaning packing fraction is equal to 0.74. So, only when you have ideal system like this, you will have the highest possible packing fraction of 0.74. So, this is also and in that case it will be called a Hexagonal Close Packed structure which is HCP.

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

Now, let us remind us what the Pearl Navarro stress was Pearl Navarro stress is given by this equation where b is the if we write in planar spacing then this will become a so w is a by 1 minus nu. So, a becomes plane planar spacing. So, if you want tau p n to be small what do we want with a, a should be large. So, you can see if it a is large this being a negative quantity tau p n will be small. So, a should be large and this happens for basal plane.

So, this is basal plane assuming ideal condition ideal HCP. Now if the a and let me call it now a i. So, basal plane now if a for any HCP which is not ideal system a is greater than a ideal then it means that the planar spacing is larger than what we are expecting in that case basal plane basal slip more preferred and as you keep reducing a. So, if you go less than a basal slip will the spacing between basal slip will not be as large as we wanted.

And some of the other spacing between some other planes if for example, the prismatic planes may become larger. And therefore, those may start to become the dominating shear stress or that they will be the more preferred slip plane. So, basal slip not as much preferred. And we look at the values of shear stress. But right now, let me show you what it does to the when does c by a value changes; however, different planes become preferred.

So, let us look at so here I will put c by a ratio and remember the ideal value is 1.66 and very few metals actually show this ideal ratio. And here I will be putting tau CRSS value for different slip systems. So, one of them is the basal which is what we are more is most interested in because we said this is what is the preferred system for ideal system for a ideal HCP. Or the close packed structure or when the c by a ratio is greater than the ideal value. Then we will look at prismatic which is the second most preferred one then pyramidal and the c plus a type.

So let us list out some of the elements metals cadmium is one of the hexagonal system zinc is another one, magnesium is another one, zirconium is another one, titanium is another one and beryllium is another one this is not the exhaustive list. But we are just comparing here some of these values. So, what are the c by a values and as you will see I put it in a descending order and these values have been taken from the book by Holland Beacon and some other values are also taken from the book by Y Chai and William Dynix which are given in your references if you look at the course hand out over there they are mentioned as references.

So, if you look at this, we see that in this particular list only magnesium comes closest to it 1.633 and the elements on that above it have c by a ratio higher than 1.633 and below this have c by a ratio lower than 1.633 which we said is the ideal ratio. So, now, when it is higher than what would what would we expect that the tau CRSS for basal slip is very very small the or the smallest and it does. So, happens it is less than 0.1 and all these values and in mega pascal even zinc is less than 0.1 mega pascal. And if you go to magnesium it is a little bit higher. But is still in the same range when we go zirconium it is much higher than the all these 3.5 and titanium is 3.1.

Now, here are some you can say discrepancies because 3.1 is the calculated value and the measured value are actually much higher 80. But we are just putting some values which are falling in the trend, but you should remember that there will also be 80 which is the experimental value and this is beryllium which is 5. So, clearly you can see that as the planar spacing with of the basal planes is decreasing the tau CRSS values are increasing meaning it is no more as easy a slip system or as easy a glide plane.

Now let us look at some of the other ones now here all these data are not available. So, we will put only the data we have again the most of these values are from two big two books which I mentioned earlier. So, what do we see here that the prismatic slip tau CRSS for the prismatic slip keeps coming down or at least that is the trend from whatever values. We have 40, 21, 12 and you were here also pyramidal values here the ratio was very high point 1 to 7. But here the ratio is much lower 3.1 to 4.2. So, even the pyramidal slips are becoming a little bit more easy as we go from c by a ratio very high to very low.

So that is the slip system preference based on the tau PN values. Now let us look at what are the possible burger vectors. So, we have seen c and a, but those are only when we have the full dislocation. But there is also a possibility of partial dislocations as we would see which is similar to what you see in our FCC system. And not only that similar similarity to FCC does not end over there. In FCC if you remember we talked about thumb (Refer Time: 17:20) tetrahedron which gives you all the possible slip planes partial dislocation burger vector and so on. And here also you have something called a bi pyramidal system which is able to describe all the possible burger vectors not the slip planes, but all the possible burger vectors. So, let us first see where does that come from.

So, again I will have to draw the hexagon and now let me put atoms. And remember there is a atom also at the centre here and what else we this is not all of it you remember I said that there are three more there is another layer in between three more atoms. So, the way we will place it this will if you make a triangle over here. There will be six triangles out of which if you look at it three of those triangles alternate triangles will contain those atoms.

So, let us say one of them is over here in between this one. So, this is one atom over here now if this is the one that is already covered then there we should have another one over here. So, let us another atom over here and; that means, the third one will have to lie over here. So, these are the three atoms over here ok. So, now, let us call this as point A this as point B and this as C. And let us call this the atom over here as S. So, now, we will be able to make you can say single pyramid no it is not a tetrahedron because not all the sides it is not 60 degrees. So, we will draw something which will look like this so we will say AS so, this is A this is B and this point is C and over here we will draw it is at the centroid. So, from centroid will connect all these. So, this becomes s. So, this is one half of the pyramid. But now that is not the complete picture when we when we want to describe all the burger vectors. Because this is not at 60 degrees this line is not same as this line these are different. And therefore, we will have to describe it separately. So, here comes another pyramid which goes below it and it looks like and here we will call it T.

So, now, we have ABC and on one top one side we have S other side we have T. And the when you connect S and T it intersects at a point which we will call sigma. Now all these points will become important when we try to describe the various possible burger vectors. So, let me also draw. So, ABC if you look at it that will be a equilateral triangle. So, ABC will look like this we are looking from the top something like from the S.

And therefore, this S and T they will fall at the centroid of this equilateral triangle. So, S sigma and T if you are looking in a projection view all of them lie at one point. Let me use a different colour so this is the projection view just to make the picture more clear I have put it like this. So, what do we get from this all this construction in HCP that is the useful thing that we can now write what are the burger vectors in terms of this. And we know with respect to this drawing with respect to the hexagon that we have over here.

So, now, let me write the burger vectors and there is a category. So, this is first let me write for perfect dislocations. Now even in perfect dislocations you would see that there is not only one possibility there are more than one possibility which we have already seen. And now we will write in terms of these alphabets and their negatives. So, that becomes so although there is 3, but when we add negatives it becomes 6 then the other categories can it be ST and TS. This is ST and the inverse is TS which is the C type of burger vector that is also one full burger vector for a full dislocation.

Then there is something called as SA slash TB which is something you can say from the centre of ST to the centre of AB that kind of vector is called ST slash AB. And since there are a so many possibilities SA SB SC TA TB TC and then AB BC CA. So, it will intersect all of those and therefore, you will get including their negatives you will get 12 possible burger vectors. So, these are the perfect dislocations. Now let us look at the possible partial dislocations.

So, how do we so here in brief what we are doing is we are connecting all the end points AB, BC, CA, ST, TS. And when you for the SA, TV you take again you take the full vector over here. And the TB the both of them are full vector and you connect them what you get is a vector called as SA slash TB. So, all of these are connecting end points, but when we are talking about partial dislocations one way or the other they will be connected with sigma. So, what are those first you can connect only the AS. So, this will become AB sorry A sigma B sigma C sigma. And the negative which means sigma A sigma B sigma C so this is 6 now. This can also be connected to S and T.

So, it is S sigma T sigma and the negative which is sigma S sigma T. So, this is another 4 burger vectors and other than that you can also get burger vectors. So, this is also connecting end points, but this is as you can see this is not a full vector AS, BS, CS, then AT, BT, CT and the negatives. So, it will become SA, SB, SC, TA, TB, TC. So, these are 12 burger vectors.

So, you see all the possible burger vectors that are there in HCP can be listed using this by pyramidal structure. And the similarity with a FCC does not end here as we will see that even the dissociation into partial dislocations do happens. And you can draw the cartoon similar to what we have in the FCC system. Now that we have mentioned the burger vector here. So, it is also imperative that we compare their magnitude and their energy vectors.

So, let me put a comparison of various vector magnitudes and their energy because energies are what will tell us which one is more preferred. And as you will see clearly that a vector is when you are talking about a perfect dislocation we have like I have said that basal slip is preferred and therefore, in the basal slip you have the A burger vector and that will have the smallest energy.

So, that is something we can we are expecting. Now let us see if it actually comes out like that. So, let me write the type and over here we have comparing first the vector then the magnitude and then their energy. So, type when I say it can be AB type. So, you can see in the previous one that there are six different types 1 2 3 4 5 6 actually 7 different types. So, we will compare all these 7. AB type which is 1/3 1 1 bar 2 0 then we have the TS type which is the C vector then we have the SA TB type.

So, this is this is what we in other words we were what we were describing as C plus A vector this is what this is represented as SA TB and then comes the partials a sigma type and right now I have not told you what should be the burger vector. But here I am writing directly and next will come when we talk about the partials then you see this form.

But then, I have also showed you the pyramid and from the pyramid you can directly find out that this is what the vector would indeed be. So, these are the partials on the left hand side we have the full dislocations. So, now, let me so as I have already given you the vectors this is just the form of the vector. And you this is like I said from the bi pyramid you would be able to directly get these vectors. And we have listed all the possible different perfect dislocations and partial dislocations. Now what is the magnitude we know this is nothing, but a.

So, the magnitude of this one is a. What is this magnitude this is c. But here for the sake of comparison we want to convert all of these to A. So, what we will do is well assume an ideal HCP system. So, assume ideal HCP system where C is equal to root 8 by 3 A. So, this automatically means that says we want to compare in terms of A. So, this becomes root 8 by 3 a. Now this is c plus a. So, we will actually it is not really c plus a as you would see this is c square plus a square over 1 by 2 and this will if you look at it, it will come to root 11 by 3 times a.

Now what is this, this is a partial burger vector and this is nothing, but a by root 3. This is again in a partial burger vector which is half of the C vector is equal to c by 2. And therefore, you can write it as root 2 by 3 a and this last one is not so easy to come or derive it, but you will have to take my word for this that this is a square by 3 plus c square by 4 1 by 2. Now let us compare their energies. So, for energy we know and we are not talking in terms of absolute values we are only comparing the relative values. So, what we do is just take the square of the magnitude of the burger vector.

So, whatever we obtained here we multiply we square it. So, this becomes a square this becomes 8 by 3 a square this becomes 11 by 3 a square so this is for the perfect dislocations. Now we have the partial dislocations a square by three, this is two by three a square and this is a square. So, first things few things to note over here that when you are talking about perfect dislocations AB has smallest energy AB type vector not just a AB has smallest energy. You can see these are much higher than that. Now when we are talking about the partial dislocations which has the smallest energy you can see that this one a sigma type vectors are the smallest.

So, we have perfect dislocations and partial dislocations and another very interesting thing is that your AS type partial dislocation. This one as you can see has similar energy as that of a full dislocation has same energy as AB type full dislocation ok. So, this is clearly AB types dislocation are much preferred when we are talking only about the partial dislocations. But even now here we come to we move on to the next part which is about dissociation of these dislocations in HCP.

$$AB = A\sigma + \sigma B$$

So now, we talked about AB type dislocation now in I will use those notation. And what is found is that even AB type of dislocation dissociate and they dissociate into what A sigma plus sigma B and they end up with stacking fault remember in the FCC. So, so yes here also we will get stacking fault what is that type of stacking fault. Let us see if we can or how we can relate to the FCC type of stacking fault. So, remember in FCC we had ABC ABC type plane in HCP we have AB AB type plane. So, let us look at the AB AB type plane. So, let if you write it down the AB AB type plane should be like this.

So, this will keep on going, but if you end up with any particular plane where you have this dissociation. So, in this particular case let me say that or you have a dislocation somewhere over here or the dislocation glides such on this plane. So, these are our basal planes AB AB all of these are basal planes here one plane another plane. So, one of these planes will have one star dislocation glides this one part of this part of this plane would have glided over the layer below it. And therefore, something will change what changes. So, let us say this is the plane which does not which remains as it is remains intact. And these are the and this is the plane and everything above it then what will happen this because it has formed a partial dislocation.

So, this much layer would remain as it is and after that what you will see is that instead of this a layer will become C layer B layer will become a layer. And therefore, you will end up with CA CA type of plane. So, this is the plane over which glide took place. So, after glide this is the form of stacking fault that you would observe and remember we are talking about these are your planes if you look at it these are your planes and your dislocation is like this. So, probably your edge dislocation extra half plane is somewhere like this it is gliding. And therefore, in the glide when it is gliding then it will create a stacking fault. So, everything above this.

So, this is the extra half plane region everything in this side will change it is position and this is only happening when we are talking about the formation of partial dislocations. So, the A layer has become C and the B layer has become A. After this partial after glide and formation of partial dislocation ok. So, now, let us come back to our this original equation which is which describes the formation of the partial dislocations AB plus sigma B and it will be useful if we just go back quickly to look at what this means.

So, here is this triangle AB has dissociated into A sigma and sigma B. So, this is what is happening and I will show you again that this is exactly same if you look only in this plane. The exactly same as what we saw in FCC system. For now just based on that diagram and based on the burger vector I have already described to you should be able to write down all the burger vectors here. So, here it will become 1 1 bar 2 0 transforming to 1 by 3 1 0 bar 1 0 this is your A sigma and sigma B will be 1 by 3. So, this is the perfect dislocation if it had moved just that way then there will be no change in the stacking fault. But since partial dislocation has formed this is the kind of stacking fault you end up. And let us now that we have written the equation. So, why not calculate the energy and remember AB has energy of the type a square A sigma has the energy of the type a square by 3. So, sigma B also a square by 3.

So, when you sum it up it becomes 2 by 3 A square. So, this is certainly lower energy implies it is favourable to form. So, it is not that it will even energetically it is possible to form it is not just theoretically what we have shown here. Here we are showing that energetically also this is feasible. So, it has lower energy. So, it will tend to form.

Now, talking about similarity to FCC where we had a by 2 1 bar 1 0 slip occurring on 1 1 1 plane. So, how is it similar? So, if we were to draw the plane atoms on this plane. So, let us call it layer A and we have another layer somewhere here. And it is and I am intentionally drawing it a little bit smaller in size although it will be of the same size. And will be touching this is just. So, that we can draw or clearly show how it is how the transformation is taking place. So, this green layer is layer B.

Now, if we if it were a perfect dislocation what would have happened this would have moved from over here to over here, but this is not what is happening it is forming a partial. So, what is that partial this is like this and over like this. So, your dislocation which is this which is given by the burger vector a by 3 1 1 bar 2 0 breaks into two partials. And let me draw it more accurate because like I said this should be exactly same. And therefore, it should be a 30 degree angle in the FCC also we get it at 30 degrees here also we get it at 30 degrees those partials because you can see the plane is similar at this level of plane when you look at things it will look exactly same.

So, this will be your a by 3. So, these are your bp 2 and bp 1 and if they were moving apart this is how it would look like. So, this will be the region where you will have stacking fault created and this will be your perfect crystal this would also be your. However, with even though with so much similarity there is still something which is different over here in this when we are talking about HCP and that is because layer A is a little bit different from layer B. So, now, if you are talking about this let us draw this again and assume that.

So, in this particular case we assumed that the dislocation layer B glides over layer A ok. But in HCP because all these planes a and b are not exactly same. We can have the other situation where you have ok. So, here what we what is different is we are saying that layer A glides over layer B. Therefore, your full dislocation is from here to here. So, full dislocation is still the same, but now the partials are actually like here ok.

So, if I draw it the partials are. So, this is your a by 3 which means that this particular when you look at the bp 1 and bp 2. Now their positions have interchanged. So, the burger vector for the first one is this one and the second one is this one. So, this is something that is different when you have HCP system here. The layer B was gliding over layer A and here layer A is gliding over layer B ok. So, before we close the chapter about the hexagonal systems there are a few points.

That I would like you to keep in mind one of the first thing is how we said that basal slip and then the prism slip prismatic slip is what is preferred. So, overall basal plus prismatic how many do we get slips independent slip system four independent slip systems. But if you look at the von mises criterion there should be at least five independent slip system for homogeneous deformation of a polycrystalline material ok.

So, it means that most of the time it what is there are two implications that for most of the HCP metals will not show homogeneous deformation at low temperatures where only basal or prismatic is activated. And this is absolutely true whether you are talking about even something like zirconium, titanium, magnesium they do not show very good deformation behaviour they are not homogeneous at lower temperature. And even at higher temperature some of these materials do show a very good homogeneous deformation. So, at higher temperature or at higher stresses homogeneous deformation must be taking place due to must take place to do.

So, what are the possibilities that will lead to homogeneous deformation. So, there are two possibilities one that some of the other slip systems get activated. So, pyramidal or c plus a system get activated. And there is still another possibility twinning. So, we already have four slip systems, but twinning can add as a fifth independence slip system. So, twinning can lead to homogeneous and both of these things have been observed. So, people have observed that this twinning does support homogeneous deformation and in some cases there is a pyramidal slip or c plus a type of deformation which leads to which allows for a homogeneous deformation.

And this one particularly is true for high stress and particular orientations. So, these are some of the important things about HCP. So, HCP is not a very you can say deformation friendly system all the metals which fall in this category they have to be modified in some way sometimes higher temperature or you have change their c by a ratio. So, that other slip systems get activated and. So, on and then you would be able to do or get absolute good deformation behaviour. So, even though they may have very good strength ductility etcetera. But some of these things can be missing that homogeneous deformation can be missing even machine a machinability would be down because the machinability is nothing but deformation at those conditions and if those if the deform the deformation is not good so, machinability may also be down and then again one needs to make some modifications. So, that you can get good deformation behaviour.

So, we will end our lecture about HCP system here and next we will talk about two more you can say more advanced systems, one in not an great extra length. But the most complicated which is ionic system and another which is very important from a mechanical engineers point of view and a materials engineer point of view which is a super lattices or which also give rise to systems super alloys if you remember nickel super alloys there are super something called as super alloys. So, we will understand where do we get those behaviour properties from when we understand the dislocations in super lattices so.

Thank you and will see you next module.