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

Lecture - 08
Dislocation Structure in HCP

So today we come back in this module to discuss Dislocations in yet another type of system which is hexagonal systems ok. So, in hexagonal as will see, we can also have a hexagonal close packed system or the hexagonal regular system.

$$\vec{R} = u\vec{a_1} + V\vec{a_2} + i\vec{a_3} + w\vec{c}$$

So, let us start with, now when we say hexagonal you all realise that hexagonal is not really a unit cell, there unit cell is rhombus type. So, how does the hexagonal system look like? This looks like; so, there are atoms in here and there is also atom over here in the centre. Similarly there are atoms over here and there is atom in the centre, there is also another layer over here where you can save the centre of this line another centre of this line, another centre of this line. See if you combine this there will be another atom here, another atom here, another atom here there all if we are talking about a metallic single phase system they are all same atom. I am just drawing in different colours because there it is easier to see over here. So, these are the different atoms that you see.

Now, here the real symmetry if you look at it would be or the unit cell, the real unit cell would be like this. So, in here this is how. So, this is the unit cell that would be actually there and here you will have. So, this will be a 1 this will be a 2 this will be c, but then there are lot of things that this kind of unit cell misses. First and foremost the symmetry of; so, if we what we are calling as actually it should I call it b; so, this is a which is termed as a 1 and b which is termed as a 2. So, what this misses is the symmetry of a b and minus a minus b.

So, this is not captured in here not only that when we write the indices using this system then the symmetry and other properties are not easy to other you can say crystallography is not easy to visualize ok. So, we come back to this system and over here we do not use the usual miller indices, what we use is called the Miller Bravais indices. So, we will introduce.

So, in this particular system what we do is that we have 3 different. So, in the plane itself we have a 1, a 2 and a 3. So, in the plane itself we have 3 indices and of course, the fourth one which is c. So, this particular type of system we have what you can say u, v, i and. So, this is the system where whether you are talking about plane or the direction you have u, v; w is in the usual system, but here we have a third one i and this i is not independent, this is dependent on u and v as will see in just a moment. So, here the way we describe we said that there are 3 lattice indices a 1, a 2, a 3 and if you look at with respect to this then a 1 is equal to a 2 is equal to b and a 3 is now not an independent like I said, it is equal to minus a 1 minus a 2.

So, it is a dependent index, this just gives it a more you can see easy to visualize where we are really trying to point the index in a hexagonal system and therefore, any lattice point can be indicated by h a 1 plus k a 2 or since we have used u, v, w. So, let me put u a 1 v a 2 i a 3 plus w c. So, this will be the index, the way to index or point in this over here and as we have already seen that this i would be some of the other u plus v plus i would be equal to 0. So, that is the way we have defined it.

Now, as I was saying that over here we will look at using this system. Now we have let us draw just on the plane. So, over here as I defined this is your a 1. So, this is a 1, this is a 2, this is a 3. Now, what are the in this new indices in this new notation what are those vectors, say if we are talking about a 1 in a very easy way to look at it is why not draw it first in the opposite direction. So, let me draw it in the opposite direction. So, this is bar of a 1 or minus a 1.

Now, what is minus a 1 equal to? This is equal to a 2 plus a 3. So, 1 a 2 plus 1 a 3; so, if I had to find the indices what I will do is I will write a 1 how many multiples of a 1 how many multiples of a 2 how many multiples of a 2 a 3 and c; c obviously, 0 we are talking in the plane a 1 and a 2 we know they are 1 and 1. And once we have two of these indices of these 3 indices we do not need to do anything else, we simply take the sum of this and take negative. So, minus a 1 becomes 1 1 bar 2 0 and therefore, if I had to write a 1 I will write 1 bar 1 bar 1 2 0. But now one other thing this is in the in the sense of direction it is right, but magnitude wise if you look at it this we are going a 1 a 2 over here a 3 over here. So, we have a 2 1 a 3 1 and therefore, a 1 was minus 2. So, a 2 2 a 3 1 and we are going minus 2 in this direction.

Already minus a 1 and we are now adding two more. So, this is a minus a 1, this is minus a 1 this is minus a 1. So, this is 3 times of that this therefore, I will have to multiply it by a factor 1 by 3 and this and take the negative of this because I to make it simple I have taken a negative direction. Now using the same principle I can get a 2 equal to 1 by 3, similarly a 3. So, you see I have made this correction because here I was looking at a 1 so I have drawn it in the negative direction.

So, a 2 and a 3 are 1. So, a 2 and a 3 are 1 and a 1 is the sum of this a negative. So, this becomes minus 2 and this is equal to the minus of a 1 because I have drawn it in the negative direction and like I said it is minus a 1 and then another two of the a 1 makes it another two in this direction minus 2. So, this is 3 times minus a 1 and therefore, if I really want to get the magnitude I must multiply it by 1 by 3.

Because this magnitude is actually 3 times of a 1 minus a 1 therefore, a 1 is equal to 1 by 3 similar using the similar methodology, if you look at a 2. So, this is the a 2 this will be 2 others are minus and this is the whole thing is multiplied by 1 by 3. So, that is the way to get a 1 a 2 a 3. Now we have this let us look at some of the simple planes and directions for the HCP system, now you know ok. So, even before I go. So, this was the direction. So, now, let me also describe over the plane before we go to the planes.

So what do we do about the planes? Just like in the cubic system what you have to do is if you are talking about any particular plane. Now let us say that there is a particular plane which is over here. So, let us say this is the plane that I am talking about and first you have to describe which are your a 1 a 2 a 3. So, this is my a 1 this is my a 2 this is my a 3 and this is my c direction.

So, again what you do here is you what you do is first find out what is the intersection on a 1 a 2 a 3; two of this is sufficient again and then you take the reciprocal of that. So, over here for example, in the a 1 direction this is so we have to. So, if we are said a 1 and a 2 are 1 then a 3 will become automatically minus 2 and c will become a sorry, here we do not need to do the a 3 will do it once we are taken the reciprocal. So, 1 by a 1, 1 by a

2, 1 by a 3, 1 by c and c is 2 1 by 2, it is intersecting at half the length now this will become reciprocal of this is 1 1 1 and then the sum of these two must be all this three must be 0. So, this becomes bar 2 and this is 1 by 2 so this becomes 2. So, this will be a 1 1 bar 2 2 type of plane.

Now, let us look at various possible planes and direction, here we will also classify what are the different planes and directions. So, the first one let us say let us talk about basal it is one of the most important planes with respect to HCP.

Now, this is one of the direction that we are interested in; and what is the plane we are interested in? We are interested in this plane and we will keep our a 1 a 2 a 3 just like the way we described earlier. So, this is a 1, this is a 3. Now since this is parallel to the plane so; obviously, a 1 a 2 a 3 are all 0 and the only direction that will lie over here would be in the c and therefore, it will be equal to 1.

Therefore, this is much simpler we are talking about 1 by a 1, 1 by a 2, 1 by a 3, 1 by c and since the intersection there is no intersection in a 1 a 2 it is equal to infinity. So, 1 by infinity 0 0 and this is sum of this is 0, this is 1. So, it remains 1 and therefore, the plane is 0 0 0 1. Now, what is this direction? This direction is nothing, but the negative of a 2 and what was a 2? Now we remember.

So, this direction that we are talking about this is negative of a 2 and simply we can write 1 by 3 1 bar 2 1 0. So, this is one of the basal planes, another basal plane that is possible in the system is let us draw it over here using a different colour. So, this is called a Basal pyramidal plane. So, this will be like this. So, here again now we are interested in where is it intersecting on a 1 a 2 a 3 and c, now c it is intersecting at half therefore, 1 by c will become 2, a 1 it is intersecting at 1.

So, it becomes 1 by 1, a 2 it is intersecting at infinity. So, it will become 0 and since we already have two of these so, 1 and 0. So, the third one has to be such that the sum becomes 0 therefore, this will become 1 0 1 bar 2 and therefore, the plane this that we are talking about is nothing, but 1 0 bar 1 2 this is the pink plane and this is this maroon plane.

Ok. So, now, let us go to still another plane which will, which is called as prismatic. So, when we are talking about the HCP system, let us also look at what is a prismatic plane.

So, this is again another HCP system and we are talking about prismatic plane. So, where is the prismatic plane over here? There are again two different prismatic plane. So, first one let me draw with this blue colour. So, this is one of the and just to remind you again this is a 1 this is a 2 this is a 3 and this is the c direction this is what is called as first order prismatic plane.

What we are interested in are the reciprocals. So, a 1 it is intersecting at 1. So, 1 reciprocal of this is 1 a 2 it is parallel to that. So, this becomes infinity therefore, one over infinity is 0. So, now, we have 1 0; so, this becomes 1. Now, this 1 this is again parallel to c therefore, it is infinity 1 over infinity is 0 therefore, this plane that we are talking about is 1 0 bar 1 0.

Now, let us draw another plane which is called the second order prismatic plane and it is this one. So, all this prismatic planes are parallel to the c direction ok. So, this is now again look at this; so, this is called second order prismatic plane and now when we are talking about intersection. So, it is intersecting at 1 on a 1 1 on a 2. So, the reciprocal of both of this is 1 and 1 and therefore, the a 3 which should be the sum negative of sum of these two should become the like this and this is parallel to c.

So, this remains like this which means this is 1 1 bar 2 0; now at this point 1 may ask is this not a possible third prismatic plane and you should answer why it is not. So, let me tell you this is not a third order prismatic plane. So, it is for you to find out why this is not a third order prismatic plane and there maybe assignment questions based on this. So, use it is will be good if you look at it on your own, now the third kind of planes and directions are which are important with respect to HCP system are the pyramidal planes.

So, what are this pyramidal as the name suggests it is inclined pyramid like. So, again this is our and where is the pyramidal planes. So, let me right the name pyramidal again there are more than one type of pyramidal plane as you will see. So, this is the first one let me draw and again a 1 a 2 a 3 and this is c direction.

So, what we are interested in again finding the reciprocal of intersection of a 1 a 2 a 3 and c, now in the a one direction it is intersecting at, so this is the a 1. So, we can say that it is intersecting a 1 and so this is parallel to a 2. So, 1 over infinity is 0. So, this becomes 0 and as far as a 1 is concerned you can say that this is 1 and once you have 1 and 0 the third one becomes bar 1. And the c direction you can see from here to here it is 1 c. So, this becomes 1 therefore, this is 1 0, bar 1 1.

Now, another plane that we will draw over here which is also pyramidal; so, here I missed out telling one thing that this is 1 over a 1 we have taken as 1 because you can consider this plane parallel here. So, this over if you are taking it here then the intersection would be at a 1 equal to 1. So, that is where we are getting 1. So, you will not take it as 0 that will be not meaningful ok. So, here again we have this is intersecting at a 1 and a 2 at 1. So, this remains 1 a 3 of course, will become bar 2 and c direction you can see it is intersecting halfway. So, there reciprocal of that will be two therefore, this becomes 1 1 bar 2 2. So, these are the two possible planes when we are talking about pyramidal.

Now, that we have looked at the different kinds of planes and directions that are possible in the HCP system. Now let us look at, we are now in a position to look at their dislocation slip system, now here again you will see that dislocations can be classified according to some categories.

So, the first and foremost thing is direction, meaning the burger type of burger vector and for each of these burger vector there will be different possibilities. So, first thing that we will look at is a, which is in which is along 1 of the a 1 a 2 a 3. So, we can write it like 1 1 bar 2 0 actually there would be 1 by 2, but we are right now concerned only on the direction.

Now, planes so, what are the possible planes? The planes are that are possible basal prismatic, all of these can contain a type of vector and therefore, they are listed here and corresponding to this we can have slip systems. So, now, that you have a direction and the plane. So, we can describe the slip system. So, far the basal it means that this is happening only in the that particular plane so this becomes 0 0 1. For the prismatic and again the direction remains the same, for pyramidal the direction is 1 0 bar 1 1 and the direction remains same because we are talking only about a type of burger vector right. Now and you can see that there is a continuous certain type of progression and that would be much more clear when we look at again what we will need to look at is the different planes that are being described over here.

So, what are those planes? First and foremost this is the direction burger vector which is 1 by 3 1 1 bar 2 0, this is one of the planes which is 1 0 bar 1 0, then there is another plane which is the prisma. So, this was the prismatic plane 1 0 bar 1 0, this is the pyramidal plane which is 1 0 bar 1 1 then there is a basal pyramidal plane which is which can be represented like this 1 0 bar 1 2 and of course, this is the basal plane which is 0 0 1.

So, these are the different you can see this is the direction and all this planes this one this is basal plane 0 0 0 1, 1 0 bar 1 0, 1 0 bar 1 1, 0 bar 1 2 and 0 0 1 they all contain this particular direction and this all can lead to a type of dislocation slip system.

So, let me just finish with the last type which is possible which is c plus a and there is only one type of plane pyramidal, but then there are 3 types of pyramidal possibilities as will see. So, the slip systems; so bar 1 2 3 is the c plus a type of slip system and as will see this is the, where is the c plus a. So, this is as the a direction this is the c directions. So, c plus a direction is nothing, but this one and this is 1 by 3 bar 1 bar 1 2 3 and where are the planes, we will see the planes right now. So, this is the first plane that we talk about is this one, this is one of the pyramidal planes the other one is this 1 and the third one is this 1.

So, this 1 is 1 1 bar 2 2, this is 2 bar 1 bar 1 bar 1 and this already we have already derived earlier. So, I am not going into it again this is 1 0 bar 1 1. So, these are the 3 different systems and will come back and discuss more about this slip systems a little bit more and then we will talk more about the dislocations in HCP and the possible stacking faults in the HCP system. So, we will end our lecture with this.

Thank you.