Introduction to Materials Science and Engineering
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Lecture – 11
Miller indices for planes

In the last lecture, we discussed miller indices for directions. Now we will take up miller indices for planes.

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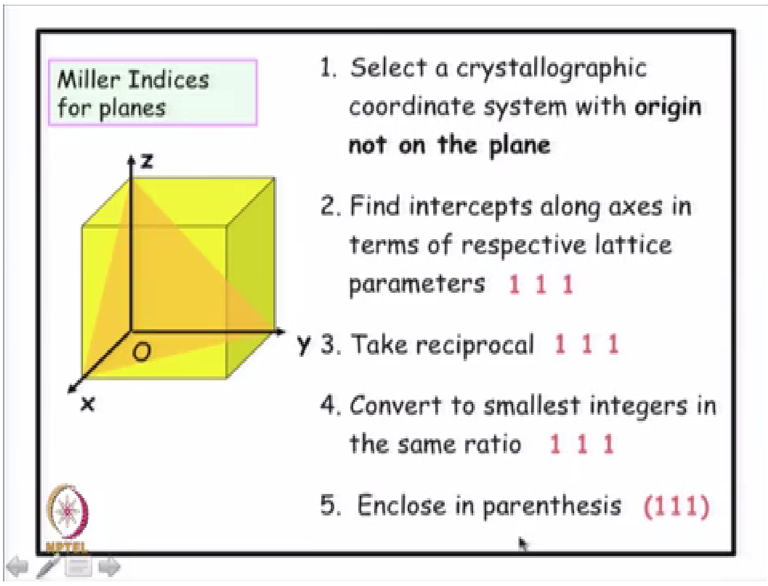

Let us look at an example a unit cell, it looks like cubic here, but it need not be cubic. In any unit cell we have a plane shown in the triangle here, which is passing through 3 corners of the unit cell and we want to specify give a name or give a miller indices to this plane. Like in the direction we have to choose an origin and a coordinate system with a crystal coordinate system and recall that the crystal coordinate system has, it is edges parallel to the unit cell edges.

But 1 difference is there when we talked about the direction, we said that the origin should be so chosen that it relies on the direction the origin for the direction is relying on the direction, but in the case of plane just the opposite is true. We have to select a crystallographic coordinate system with origin not on the plane this point has to be kept in mind. It will become obvious why this requirement is there? We choose a origin here in the back corner which is not 1 of the corners through which this plane is passing and we set up the XY and Z axis which are parallel to the unit cell edge. This is the first step and it is an important step beginners can make a mistake by choosing origin on the plane. We have to keep in mind that origin should not lie on the plane, if we are trying to find the miller indices of the plane.

The second step is find the intercepts along axis in terms of the respective lattice parameter. So, this plane is intersecting the X axis at the unit cell corner, which means it is intersecting at a distance a. A is the edge length of the unit cell along the X axis, but we will show this as 1 because we are trying to write the intercepts in terms of respective lattice parameter in particular for this plane I have selected that all the 3 intercepts are 1 1. So, we have 1 1 1 as the 3 intercept the first intercept 1 says that the plane is intersecting at a distance a from the origin the second 1 tells us that it is intersecting at a distance b from the origin and the third at the distance c from the origin.

Then we have 2 more steps for completeness we write it here although; we do not need it immediately and it is an important step that the intercepts are then reversed or you have to take the reciprocals of the intercept,intercepts directly are not taken as miller indices, but the reciprocal of the intercepts are taken as miller indices in this case of course, it is trivial because, we have a started with the simple plane all of whose intercepts are 1 1 1. So, taking the reciprocal it still gives me 1 1 1. The 4th step is to convert again them into small integers having the same ratio we had this step for the direction also the same step we repeat here for planes as well.

So, if we had any fractions or if we had any common factor we would have cancelled them suitable by multiplying or dividing by some number again that step is not relevant here for this example. So, we simply write it as 1 1 1. The final step again an important step is to use the correct bracket and in this case, we use parentheses that are the round brackets for directions remember we used square bracket; now for planes we are using round bracket. These conventions we need to follow.

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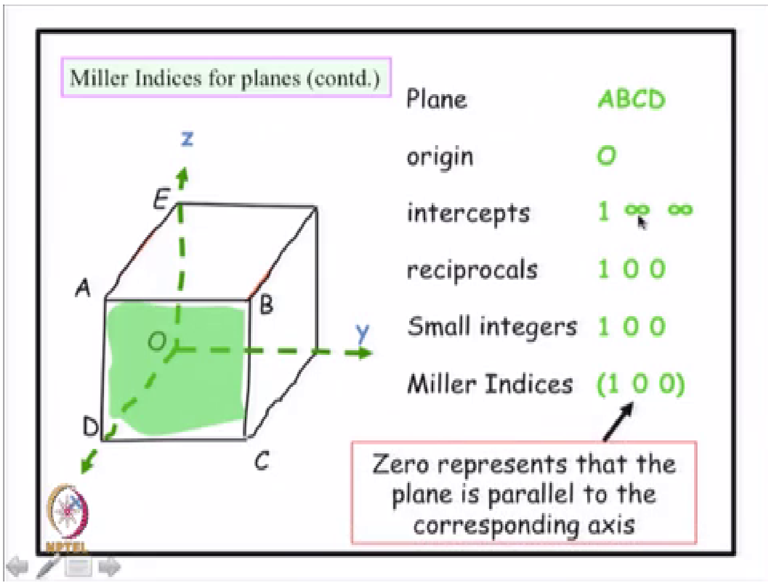

Let us now look at another example. Now, we want to index this front face of the unit cell the plane ABCD. So, we choose an origin on the back face corner the XY and Z axis are there. So, origin at O not lying on the plane and then we find the intercept look at this plane it is intersecting the X axis at 1 or A. So, the X intercept is 1, but this plane being the front face of the unit cell is parallel to the other 2 axis. It is parallel to Y and parallel to Z and whenever a plane is parallel to any given axis v by convention take the intercept as infinity. So, if the plane is parallel to axis y we assume that it is intersecting the Y axis at infinity. So, we will write the intercepts here as 1 for the X axis and infinity for both Y and Z because it is parallel to both Y and Z.

Now, taking the reciprocals become relevant because when we take the reciprocals of infinity we put 0s and finally, they taking it into small integer it is already small integers there is no common factor or there is no fraction. So, I still get 1 0 0 and finally, the miller indices I put the round brackets could be find that it is miller indices of a plane. So, this green plane will have the miller indices 1 O O and please note that 0 corresponds to 0 in the miller indices correspond to infinity in terms of the intercept and infinity in terms of intercept means the plane is parallel to that axis. So, a second 0 means that a plane is parallel to the Y axis the third 0 means plane is parallel to the Z axis.

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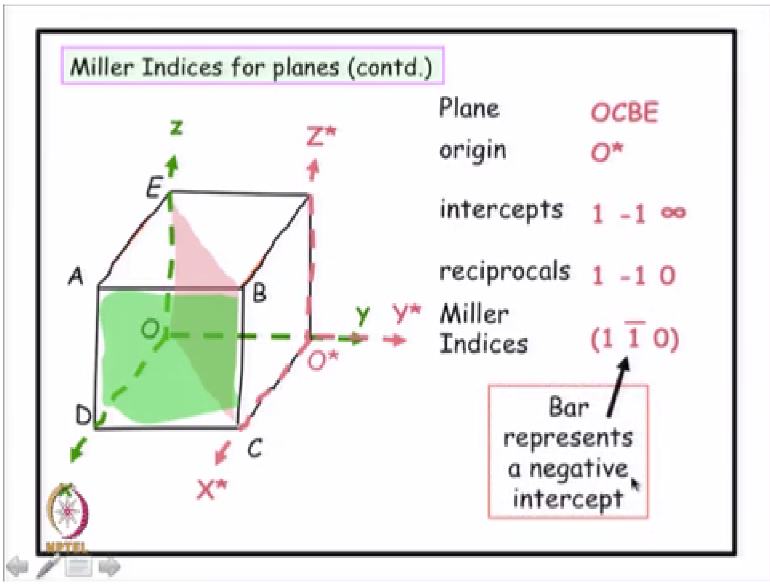

Now let me introduce another plane in the same unit cell; this time the plane OCBE now this plane happens to be passing through my chosen origin. So, the first condition the very first condition that plane should not pass through the origin is being violated. I can remedy this situation by shifting my origin which is allowed crystallographically. So, I take my origin to another corner which is not passing through the plane or which is not lying on the plane. So, I shift my origin to this corner. Please note that when I am shifting the origin to this corner, I am keeping the axis parallel this is what we had done for the directions also and the same procedure has to be repeated for planes as well.

So, we are free to choose the origin anyway, but once for a given problem, if we have chosen the axis orientations then the same axis orientation has to be followed with the new origin. So, my X is star axis is parallel to X the Y star axis is parallel to Y and the Z star axis is parallel to the Z direction because, I want to relate the miller indices of this new plane to my original plane ABCD. So, the intercepts now on the X axis the intercept is 1 on the y axis if I move in the positive direction there is no intercept to get the intercept on the y axis, I have to move in the negative direction; so I have a negative intercept in the y axis and if the plane is still parallel to the Z axis. So, the third intercept is infinity.

We now take the reciprocals. We get 1 minus 1 and infinity the reciprocal is taken as 0. We now put the miller indices into round brackets and just like for the direction we write the minus as a bar over the number. Wherever we have bar means we have a negative intercept.

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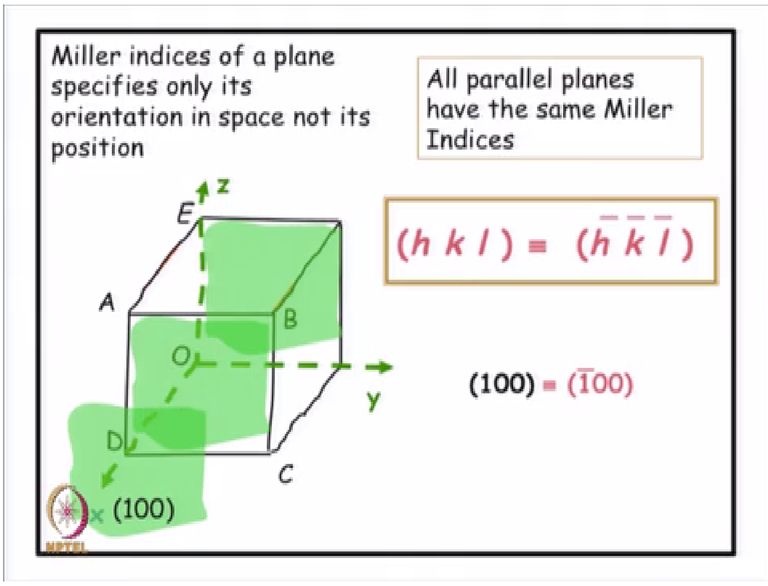

Let us make this point that whenever we write miller indices of a given plane actually it is not representing only that plane, but all parallel planes. Miller indices of a plane is specifies only it is orientation in space and not it is position. It can be any plane parallel to a given plane. So, when I say 1 0 0, I did it for the front face of the unit cell, but the back face also will become 1 0 0 and all faces parallel to this will be 1 0 0. So, all parallel planes have the same miller indices and in fact, we also have the convention that if all indices are multiplied by minus 1.

That if all of instead of the indices h k l if we take the negatives of them minus h minus k and minus l or bar h bar k and bar l then they represent the same plane. This is true because we are free to choose the origin and these 2 indices depend on which side of the plane we have chosen the origin. Note that any plane will give divide the space into 2 half we are not allowed to choose the origin on the plane. We can only choose the origin on 1 side 1 half of the plane or the other half of the plane. So, when we choose the origin on 1 half space, we will get 1 set of indices and if we choose origin on the other side, we will get the negative indices.

So, for example, the 1 0 1 0 0 and bar 1 0 0 actually represent the same plane. There are situations in which we may like to distinguish between these, but this is the useful convention.

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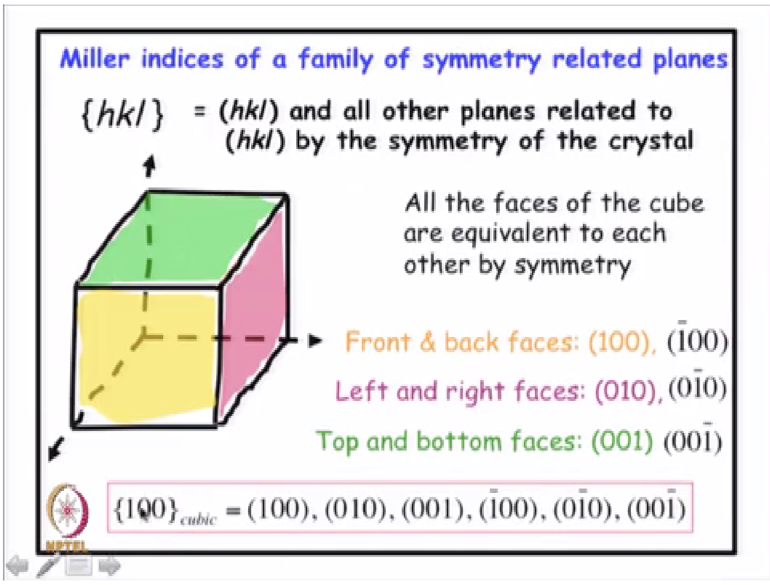

Now, just like we saw that there are symmetry related directions and there was of interest to represent them by 1 set of miller indices all symmetry related directions, similar convention or several similar requirement is there for miller indices of symmetry related planes. If we have a set of symmetry related planes then we put them 1 of the indices we put them in angular brackets. Sorry not angular bracket, curly bracket. So, if you use this curly bracket it represents not only the h k l plane, but all other planes related to h k l by the symmetry of the crystal. So, for example, we know that by symmetry if I have a cubic unit cell by symmetry all phases of the cube are equivalent they are symmetry equivalent because they are symmetry of operations of the cube which will take 1 face to the other.

So, let us look at the front and back faces. So, we have 1 O O and bar 1 O O then we have left and right faces. So, this is O 1 O and O bar 1 O and finally, the top and bottom faces. So, O O 1 and O O bar 1 and if we want to represent all these planes in 1 set of miller indices I pick up any of these 6 as the representative member and put it in the angular bracket. So, if I put 1 O O if I pick up 1 O O as a representative of all these planes then it means any of the 6 indices 1 O O O 1 O O O 1 bar 1 O O O bar 1 O and O

O bar 1 recall that since these are representing symmetry related planes the meaning of this indices symmetry related direction indices, the family indices will depend upon what crystal symmetry we are talking about. So, this equivalence which we have written here is only for cubic and that is why I have given the subscript cubic to 1 O O. Other crystal systems it is not necessary that 1 O O will mean all these 6 indices.

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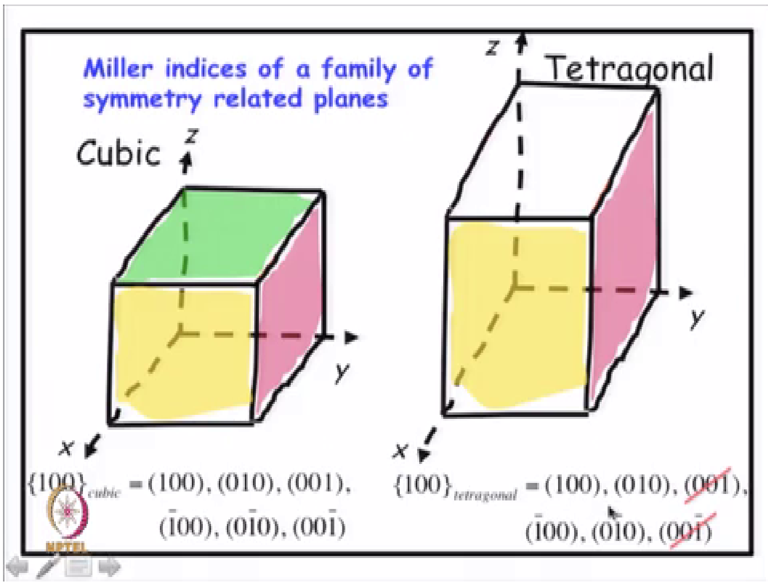

So, we will take up an example ,let us consider the tetragonal we have already seen that 1 O O cubic means these 6 indices, but what about 1 O O tetragonal 1 O O tetragonal in terms of the face is the front face of the tetragonal unit cell. This face the yellow face, but tetragonal has a 4fold symmetry axis, parallel to the z axis. So, all the vertical rectangular faces are equivalent.

So, 1 O O the yellow face is equivalent to O 1 O which is the red face here, but then the horizontal face the base of the tetragonal unit cell or the roof of the tetragonal unit cell is the 0 0 1, plane this is a square face and this is not equivalent there is no symmetry operation of the tetragonal system which will take this vertical face into a horizontal face and geometrically we can see that there cannot be any more mapping of a rectangle to a square. So, there is no symmetry by symmetry the horizontal faces are different from the vertical faces. So, when I say 1 O O tetragonal the horizontal faces are not member of that family. So, we will have only 4 indices.

Now, 1 O O O 1 O bar 1 O O and O bar 1 O I have cancelled O 1 and O bar 1 which represent the horizontal faces which were member when we were talking about sorry when we were talking about the cubic family, but in this situation they are in the tetragonal system they are not equivalent. So, it is important to keep this in mind sometimes 1 makes a mistake to assume that always any permutation of the number given will represent the family. This will be true only for cubic system because in cubic all 3 edges are equivalent. So, the numbers corresponding to those edges can be permuted in other systems we have to be careful. In tetragonal the X and Y were equivalent. So, X and Y can be permuted, but Z is not equivalent. So, the Z indices cannot be permuted.

So, finally, let us complete this discussion on miller indices by summarizing our notation.

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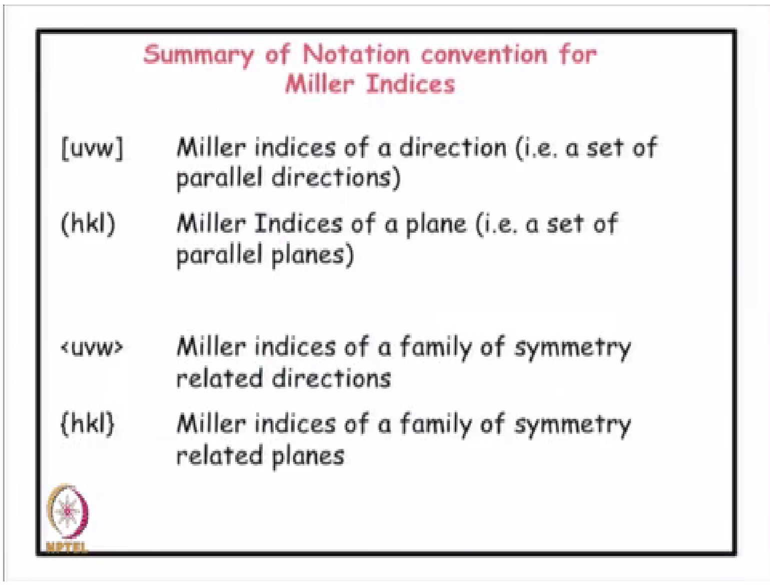

So, we have seen that miller indices for direction we used u v w inside a square bracket. Then miller indices of a single plane, we had h k l in a round bracket .if we talk of symmetry related family of directions then we use angular bracket and if we use symmetry related family of planes then we use curly bracket.

So, with this we end the discussion of miller indices.