Crystals, Symmetry and Tensors
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Lecture 2c
Miller indices for planes

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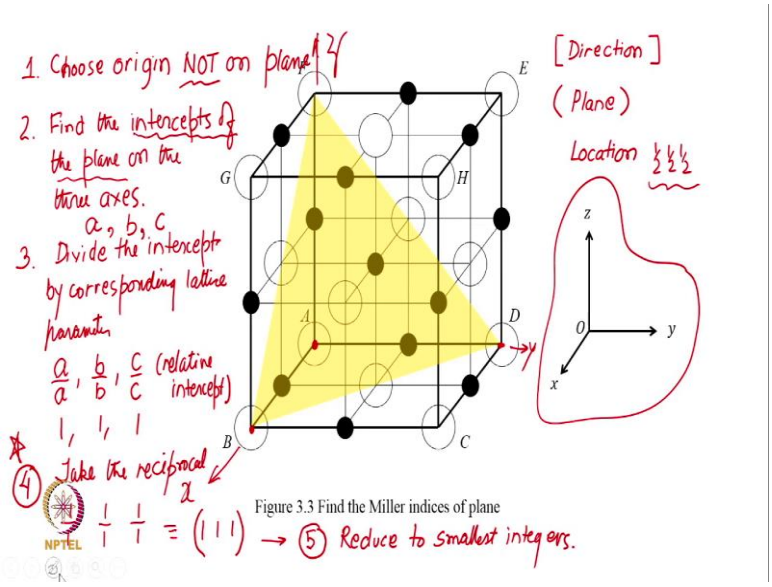

Figure 3.3 Find the Miller indices of plane

Now, let us come for plane. Plane is a little complicated and becomes interesting when we look very arbitrary, the definition for plane looks very arbitrary when we look at it from the plane point of view, but when we go into the reciprocal space and define the reciprocal lattice and reciprocal vector, which we will do in the next class, so there it becomes more meaningful that while we were defining this way.

So, here our first specification is again to choose origin. But in contrast to what we did for direction, direction we were insisting that choose on the direction. Here, we will say, choose origin not on plane if you have chosen your origin on the plane, if I choose for this plane, B or D as my origin, I am done, I will not get the miller indices of this plane, I just cannot get. Why I cannot get? Because the second step is Find the intercept, find the intercepts on the three axes. Obviously, if you choose the origin on the plane, what is the intercept?

Student: (())(01:55).

Professor Rajesh Prasad: All three intercepts are 0. Now, if I choose some other plane passing through the same origin different plane, what will be the intercept of that different plane?

Student: (())(02:06).

Professor Rajesh Prasad: Again 0 0 0. So, 0 0 0 will not be a meaningful intercept, and will not give me any meaningful information about what plane I am talking about. Every plane passing through the origin will give me 0 0 0 whatever its orientation. So, because we are interested in intercepts in defining the miller indices, we are interested in intercepts, that is why step 1 is justified that you do not choose your, or you never choose your origin on the plane. Then divide the intercept.

Again, we do that fractional thing. Divide the intercept by corresponding lattice parameter, by corresponding lattice parameters. So, for this plane, let us choose the origin A. So, then we are finding that the x axis intercept, and x, y and z I have selected in this orientation. So, from origin A x is here, y is here and z is there. And I am finding that, and the unit cell as length was A.

So, the x intercept is a, y intercept again a full b, full unit cell as length and unit cell as length is b and the unit cell as length is c where it is intercepting the z axis. So, intercepts were a, b and c. But the 3rd steps asked me to divide them by the corresponding lattice parameter, so it is the ratio. So, this is the relative intercept. So, becomes 1, 1, 1. The 4th and the craziest step is take the?

Student: Inverse.

Professor Rajesh Prasad: Take the reciprocals. Bhaiyya, intercept mill gaya uske baad bhi usko kuch or kar rahe hai thudhi zabardasti hogayi. So, take the reciprocal. So, here of course it is trivial even if we had forgotten to take the reciprocal, we would have got the correct answer. But not always, we will not always be so lucky. Here, since all were 1 and reciprocal of 1 is also 1. So, here we get this step is trivial.

And the 5th step, an important step is to put them into round brackets. And cryptographers are very finicky about the choice of bracket. So, for direction I use the square bracket. So, if you use wrong bracket, you will miss communicate in the crystallographic world and in the exam situation you will lose marks.

So, you should not for your own happiness you should be careful about the choice of bracket direction square bracket, plane round brand. It was not always so, gradually this convention developed. In very early literature you will find maybe for direction and plane both round bracket or a square bracket but gradually the system has developed and now we have to follow that.

Student: Is there any convention for coordinates, or (())(06:31) coordinates for bracket convention?

Professor Rajesh Prasad: Yes, yes, yes, we will come to that also. The exact (())(06:40) position, position of --

Student: Like we had half, half, 0.

Professor Rajesh Prasad: Yeah.

Student: -- that is (())(06:45).

Professor Rajesh Prasad: Yes. So, a particular location center of the queue, very good question. So, this is direction, this is plain, location, leave it without bracket. So, again not very uniformly followed, but quite often careful crystallographers follow that. So, they will simply write half, half, half. So, first of all it is fractional.

So, that itself indicates that we are talking of location otherwise, if it was a plane or direction I would have multiplied by 2. I am missing that step. After taking the reciprocal, again we have the, I jump to putting the bracket. If there is some common factor or if some fraction is there, so, reduce to?

Student: Inverse.

Professor Rajesh Prasad: Reduce to smallest integers that step is here also, smallest integer. And then maybe in the 6th step you put the correct bracket. So, it is clear. So, this plane is, this nice plane is 1 1 1. Again, think of this, this was a nice sodium chloride unit cell, a equal b equals c, alpha beta gamma 90 degree. So, it was a nice Cartesian system it was giving. So, 1 1 1 plane was actually intersecting at a distance 1 1 1.

Start imagining distorting this unit cell in your mind's eye. Make a, keep it orthogonal, but make a, b and c different. What will display in b then? Still 1 1 1 because cutting a, x axis on a, a by a is 1, cutting b axis on b, b by b is 1, cutting the z axis on c, c by c is 1. Now, start tilting the angles also. Axis are no more orthogonal, what will display in b?

Student: 1 1 1.

Professor Rajesh Prasad: 1 1 1. So, a plane which cuts the terminal point of a, terminal point of b and terminal point of c will always be 1 1 1 irrespective of the unit cell size or shape.

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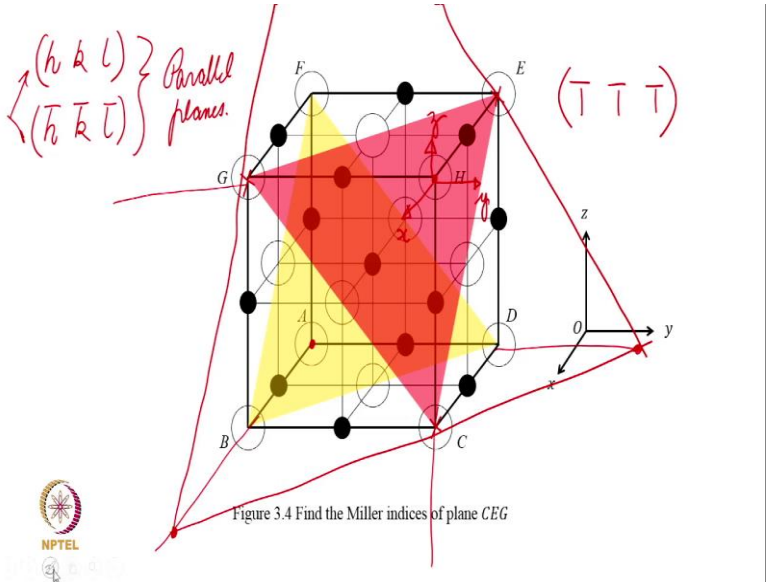

Figure 3.4 Find the Miller indices of plane *CEG*

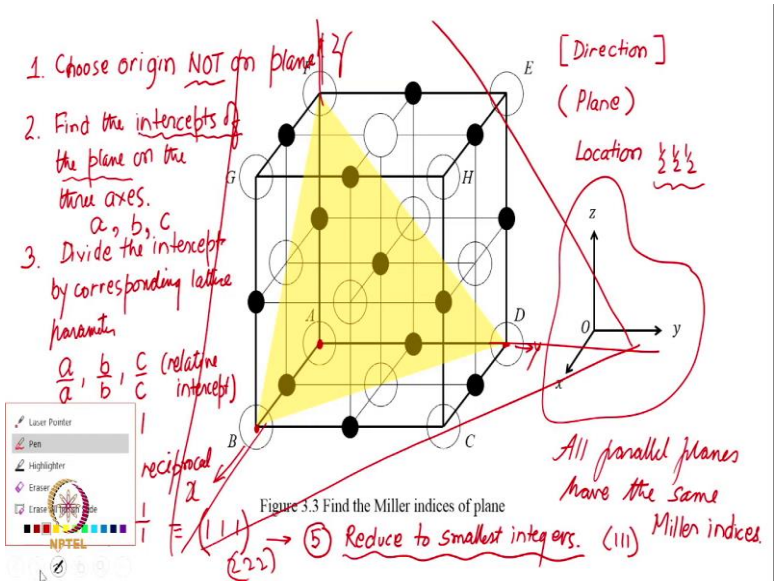

Figure 3.3 Find the Miller indices of plane

What will be the miller indices of this pink plane CEG?

Student: (())(09:40).

Professor Rajesh Prasad: Yeah?

Student: Minus 1, minus 1, minus 1.

Professor Rajesh Prasad: Yeah, because now I will choose the origin here. I will choose the origin here. I could have chosen or this origin also because that is also not lying on the plane, only thing is that I cannot choose origin, not allowed origin are C, E and G, because they are

lying on the plane, so I can choose those as origin. A I had chosen for the yellow plane, I can continue using it for this pink plane.

Only issue is that I am not able to visualize this plane when extended because the plane is plane, plane is not triangle, triangle is intersection of the plane with the unit cell. So, plane is infinite, so that infinite plane with the in finite x axis will show some intersection, but where? Either I have to be a (())(10:45), or I have to have in very good geometric visualization, or I am a computational wizard, that I can quickly calculate where this plane is going to hit the x axis.

If I am not all that, and I am just a simple chota scientist trying to figure out the miller indices, it is better to choose shift my origin to a more convenient location. And I find that for this pink one, if I choose h, then I am able to see the intercepts on all the three axes. And if so happens but as I shift, I am not allowed to invert my axes, so axes are still in the x y z direction. So, the intercepts are now opposite, intercepts are now opposite.

So, x has a negative intercept 1 bar, y has a negative intercept 1 bar, z has a negative intercept 1 bar, so bar 1, bar 1, bar 1. And these planes you see are parallel. So, it is actually a general result, that any indices h, k, l, if you have a plane, and if you make all of them negative h bar, k bar, l bar, they will always be a parallel planes. With respect to the yellow plane, where was the origin, above the plane or below the plane?

Student: Below the plane.

Professor Rajesh Prasad: Below the plane. With respect to pink plane, where was the origin above the plane or below the plane?

Student: Above the plane.

Professor Rajesh Prasad: Above the plane that is what is actually the difference between positive and negative indices. We are insisting that origin cannot be on the plane. A plane divides a space into two half. If I have a plane like this, it is dividing the space into left and right, my left and my right. I am not allowed to take the origin on the plane. So, I will either take the origin on the left or I will take the origin on the right, both sides are fine.

If I get a miller indices, for the same plane, if I get, here they are two different planes, but even for the same plane, we will see example, for the same plane, if I am choosing the origin on the left and I get h, k, l. If I go to the other side, I will get the origin or I will get the miller

indices h bar, k bar, l bar. So, 1 1 1 and bar 1 1 1 can actually be considered same because parallel planes are considered to be the same plane, why?

To have the same miller indices, that was this reduced to smallest integer. This plane was intersecting at 1 1 1. I take then the other parallel plane which intersects at 2 2 2, it is going at 2 2 2. But then I will get here 2 2 2 but the 5, step 5 is reduced to a smallest integer we will make it 1 1 1. So, all parallel planes have the same miller indices.

Student 1: Sir, according to this we should call the next one as anti-parallel plains, the next (())(14:55).

Student 2: Because they are having plain normal opposite to each other.

Student 3: No, they are parallel planes.

Professor Rajesh Prasad: Plane normal is your choice whether they are having plane normal in the same direction or opposite direction is your choice. If you are thinking of some volume within these two planes and thinking of outward normal then maybe opposite direction, but as an individual plane for the plane I can take the normal this way or this way. So, that is your choice.

So, by that argument the yellow and pink plane should have had the same miller indices. So, I could have called both of them 1 1 1. And what I was telling you that if you can work out where it will intersect, actually this is the plane which is 2 2 2. If I join this, this and this you can see that this is a smaller triangle chota triangle in this bigger triangle because of the chota triangle, I was not able to imagine where they are intersecting on the axis, but if I extend it and see where it is intersecting it is exactly 2 2 2.

So, by that philosophy it should have had the miller indices 1 1 1. Why it had bar 1 bar 1 bar 1? Because I shifted the origin to the other side, instead of choosing the origin on the same side I shifted the origin to the other side, so I got it negative.

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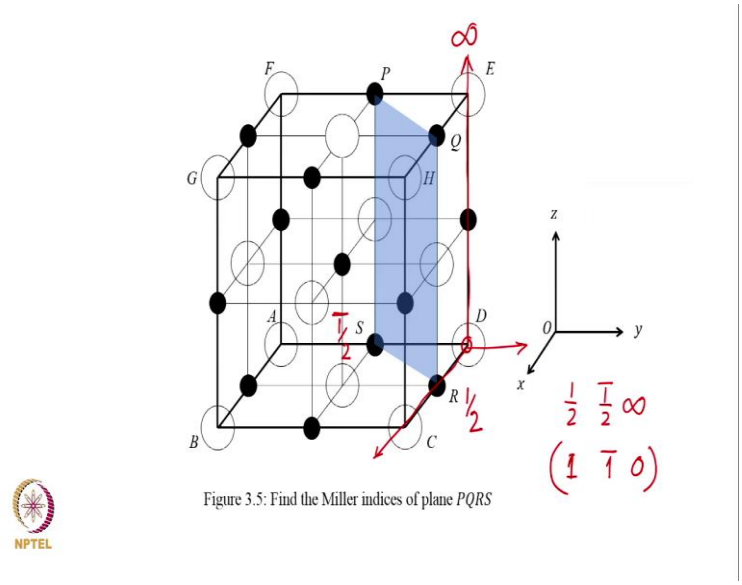

Figure 3.5: Find the Miller indices of plane *PQRS*

So, now find it for PQRS. What is the choice of origin?

Students: D.

Professor Rajesh Prasad: D, because from D only, I will be able to see the intercept. Of course, it could have been E also, D and E are equivalent. From E also I can see the intercept. On the x axis, what is the intercept?

Student: Half.

Professor Rajesh Prasad: Half. On the y axis, what is the intercept?

Student: Minus half.

Professor Rajesh Prasad: Minus half. And on the z axis, what is the intercept?

Student: Infinity.

Professor Rajesh Prasad: Infinity because it is parallel. So, when it is parallel we take the intercept infinity. So, intercepts are half, minus half, infinity, multiply by 2, 1, bar 1, 0, put it in round bracket 1, 1 bar, 0.